Dear Editor,

Hereby we uploaded the revised manuscript. We have addressed all comments from both reviewers.

In addition to the suggested changes in the rebuttal letters we have moved the discussion of the shape factors B and g^G partially to the results section, and merged section 4.1 and 4.2.

We have gathered the rebuttal letters below followed by a track changes version of the manuscript. Note that the abstract has changed significantly but these changes were not picked up in the track changes version of the manuscript.

If any questions remain, do not hesitate to contact us.

Kind regards,

Quirine Krol and Henning Löwe

Dear Aleksey Malinka,

Thank you for your detailed and careful review and the your generally positive opinion about the work. We will address all your discussion points in the following, comments are copied and replies are given in blue. We also included the additional comment we received by email. Changes to the manuscript will be documented by a track-change pdf.

Kind regards,

Quirine Krol, Henning Löwe

The article presents a study, important for optics and physics of snow. It improves our understanding of snow microstructure. The authors attract our attention to the importance of the third term of the expansion of the correlation function, related to the curvature of the air-ice interface. One of the achievements of the work is the correlations between the microstructure parameters, both short-scale and long-scale, which are established experimentally by investigating the snow samples.

There are some points to discuss.

1) The authors state that the second term in A(r) expansion (and therefore p(0)) is equal to zero and explain that this is a direct consequence of the interface smoothness. However, the widely used (e.g., by Debye) exponential function for A(r) has the obviously nonzero second term. At the same time, there are interface models, such as the Switzer model, that provides strictly exponential correlation function. Particularly, in the Switzer model the space is dissected by a set of random planes into random polyhedrons and the resulting polyhedrons are assigned to ice with the probability 1-ϕ, and to air with the probability 1-ϕ. This interface is not smooth: it has plane facets and sharp edges. Obviously, it doesn't match the morphology of aged snow, but fresh snow seems to be much closer to the Switzer interface than to smooth one, because of the facets and edges of ice crystals. With this in view and taking into account the importance of the exponential correlation function, it would be extremely desirable to discuss the facet-edge interface and its relationships with the smooth one

Reply: It is true that the second order appears theoretically if discontinuities in the structures such as edges and corners are present. Fresh snow, as we know, contains many of these features. The ability to detect this second order term and relate it to discontinuity features is however difficult due to image resolution and noise in the data. A theoretical sharp edge would be treated practically as a rounded edge, which likely shifts weight from the second to the third order term. The resolution of our snow samples is raised by the second referee (see comment 2) As discussed there, we only find a very weak bias of image resolution on the third order term. A second argument is given by the shape of the chord length distribution that tends to zero for small chords which is a direct consequence of the absence of the second order term in the correlation function by virtue of eq.(14).

Changes to the manuscript: In the theoretical section we have added a sentence that mentions the role of sharp edges of the fresh snow samples. We also added the discussion on image resolution in the discussion session.

2) The motivation of Eq. (15) looks invalid. In general, the integral of a function from 0 to ∞ is not determined by its behaviour at 0. More precisely, the authors say that "A(r) depends at least on two independent length scales, λ1 and λ2" and further "In the absence of other relevant scales…" But „at least" doesn't mean „only". It is obvious that, as λ1 and λ2 are the coefficients of expansion at 0, there are other terms and, hence, other independent length scales at the interval (0, ∞). Figure 1b clearly demonstrates the idea that the integral is not determined by the behaviour at 0, because the contribution of the function tail can be of any value. This note doesn't affect the further results of the work, because the authors show that short-length and tail scales must correlate and try to explain why. However, at the stage of Eq. (15) this statement looks ill-founded. Let me suggest the idea.

As the value of the correlation length ξ is derived from the fitting the correlation function by the exponential at the whole interval, the estimation

$$\int A(r)dr = \xi$$

looks much more reliable. Partially, this implication is confirmed by the fact that, when considering the correlation between ξ , μ_1 and μ_2 , the obtained correlation coefficient at μ_2 is higher than that at μ_1. (Minor: the differential dr is missing in the integral).

Reply: We acknowledge the ambiguity in motivating Eq. 15 in the present form, and for that reason we abandoned this argument, as also suggested by the second referee (see his comment 6).
The proposed idea is an interesting alternative to define and measure ξ. For correlation functions that are strictly exponential this definition is equivalent. This is however more in the direction of the length scale required for the microwave scattering coefficient, where the relevant scale (raised to the third power) is the zero mode of the Fourier transform of the correlation function, i.e. the volume integral over the correlation function. We will however stick here to the more "traditional" definition and estimate ξ by fitting the correlations function as done in (Vallese 1981, Mätzler 2002, Calonne 2015, Proksch 2015, Löwe 2011,2013,2015)

Changes to the manuscript: We have changed the motivation of eq.(14).

3) Page 14, line 25: "In the previous sections we found a statistical relation between the exponential correlation length and the chord length moments on the other hand." I guess the authors wanted to say "between the geometrical scales λ_1 and λ_2 and the chord length moments," because the relation between the exponential correlation length and the chord length moments is considered just below.

Reply: That is correct.

Changes to the manuscript: We have changed the sentence accordingly.

4) Introducing the factor $1-\phi$ into Eq. (24) the authors go back to the length $\lambda 1$ in the second term by virtue of Eq. (13). This is worth to note. Also, with the factor $1-\phi$ in Eq. (23) the second term turns to μ_1 . In the whole, it is worth to underline that λ_1 and μ_1 are always related with Eq. (13) and indeed μ_1 have the meaning of the optical size, being exactly $\mu_1 = 2d_{opt}/3$ independently of the snow density.

Reply: We agree that we should emphasize both, the μ_1 and λ_1 relation and its independency of the density.

Changes to the manuscript: We added a sentence in the theoretical section to emphasize the μ_1 and λ_1 relation and included the (1-φ) term in the discussion.

5) Page 19, line 18-19. "The results in Malinka (2014) are mainly based on the Laplace transform of an exponential, $p(\alpha) = 1/(1+\mu_1\alpha)$, which only involves μ_1 (or the optical radius via Eq. 1)." This is not completely true, because the exponential law is considered only as an example, though very important one. I would just delete this sentence, because it doesn't carry important information.

Reply: We agree.

Changes to the manuscript: Deleted the sentence.

6) Page 19, line 20, table 1: "relative importance $\alpha\mu 2/2\mu 1$ of the second-order term compared to the first-order term in the expansion Eq. (12)." This value doesn't look very informative. I think that much more informative will be the value, proportional to the variance α $(\mu_2\text{-}\mu_1^2)$ $/2\mu_1$, because it will give the deviation from the exponential law.

Reply: We agree that the deviation of the exponential distribution would be illustrative here. If this deviation is defined by subtracting the two Taylor series up to the second order and normalizing by the first order term, we however end up with $\alpha(\mu_2/2\text{-}\mu_1^2)$ $/2\mu_1$. Alternatively, the deviation from an exponential can be also characterized by the ratio $(\mu_2/2\mu_1^2)$, which is exactly unity for an exponential distribution. The values found here are considerably lower (this can be directly deduced from Fig. 8 of the present manuscript). Since this Figure will be replaced according to a comment from reviewer 2, the values of this ratio will be given in the Discussion. This also confirms what is already shown in Fig.5/Fig.8, namely that the chord length distribution of depth hoar is systematically closest to an exponential.

Changes to the manuscript: Table 1 is adjusted and the range of values for the ratio is given in the discussion section.

7) It would be nice to consider these relations taking into account the relationship between A(r) and p(l) in the general case of a dense medium, not restricted by the dilute one

Reply: We actually mentioned this point explicitly in the discussion. The work (Roberts and Torquato 1999) investigated this connection for Gaussian random fields, with good agreement over a broad range of volume fractions. This also indicates that the assumption of independence of successive chords (which underlies (Roberts and Torquato 1999) does not seem to be very restrictive. Their method however requires numerical Laplace inversion and the computation of another correlation function. For Gaussian random fields the latter is known analytically, but here it would require a considerable additional effort to introduce the relevant concepts and carry out the numerics, with almost no benefit for the established connections between the length scales.

Changes to the manuscript: The discussion has been rewritten and this point is made clearer now.

8) The point that was raised in the email discussion: you compare the expression A2 used by Libois et al., 2013 with the expression A3 from my paper (or eq. 23 in that numbering). But expression A2 (A1) is written for small absorption only, while eq. A3 is applicable to any absorption values. You can easily check this by the limit of strong absorption:
when $\alpha =\infty$ and $L(\alpha) = 0$, therefore $1\text{-}\omega = T_{out}(n)$ or $\omega = 1\text{-}T_{out}(n) = R_{out}(n)$, which means that all the light that goes into the particles is absorbed. This limit is not true for A2. For comparison you'd better take eq. 25 for small absorption instead of general eq. 23: $1\text{-}w = n^2\,\alpha\mu_1$ (in your notation) and easily find the B-factor $B = n^2 = 1.68$ at 1.3 um for ice. The deviations of B from this value demonstrate the difference between the models used by Libois et al. and the model of the random mixture.

Reply: We agree that the limiting case of α and to ∞ is not consistent in both expressions. However in practice we compare both expressions only in the limit of small α, for which both are supposed to be valid. This issue was brought up also by the second referee under point 2 and is further discussed there.

Changes to the manuscript: We clarified the underlying assumptions in the appendix and added necessary details to the discussion of the Figure in the discussion section.

References by the referee:

P. Switzer, "A random set process in the plane with a Markovian property," Ann. Math. Statist 36, 1859-1863 (1965).

References by the authors:

Calonne, N., Flin, F., Lesaffre, B., Dufour, A., Roulle, J., Puglièse, P., Philip, A., Lahoucine, F., Geindreau, C., Panel, J.-M., Rolland du Roscoat, S., and Charrier, P.: CellDyM: *A room temperature operating cryogenic cell for the dynamic monitoring of snow metamorphism by time-lapse X-ray microtomography*, Geophys. Res. Lett., 42, 3911–3918, doi:10.1002/2015GL063541, 2015.

Löwe, H. and Picard, G.: *Microwave scattering coefficient of snow in MEMLS and DMRT-ML revisited: the relevance of sticky hard spheres and tomography-based estimates of stickiness*, Cryosphere, 9, 2101–2117, doi:10.5194/tc-9-2101-2015, 2015.

Löwe, H., Spiegel, J. K., and Schneebeli, M.*: Interfacial and structural relaxations of snow under isothermal conditions,* J. Glaciol., 57,499–510, doi:10.3189/002214311796905569, 2011.

Löwe, H., Riche, F., and Schneebeli, M.: *A general treatment of snow microstructure exemplified by an improved relation for thermal conductivity*, The Cryosphere, 7, 1473–1480, doi:10.5194/tc-7-1473-2013, 2013.

Mätzler, C.: *Relation between grain-size and correlation length of snow*, J. Glac., 48, 461–466, doi:10.3189/172756502781831287, 2002.

Proksch, M., Mätzler, C., Wiesmann, A., Lemmetyinen, J., Schwank, M., Löwe, H., and Schneebeli, M.: MEMLS3&a*: Microwave emission model of layered snowpacks adapted to include backscattering*, Geosci. Mod. Dev., 8, 2611–2626, doi:10.5194/gmd-8-2611-2015, 2015b.

Vallese, F. and Kong, J.*: Correlation-function studies for snow and ice*, J. Appl. Phys., 52, 4921–4925, doi:10.1063/1.329453, 1981.

Dear Quentin Libois,

Thank you for your very comprehensive and careful review and the overall positive opinion. We will address your comments point by point below, comments are copied and replies are given in blue. Changes to the manuscript will be made available by track-change pdf.

Kind regards,
Quirine Krol, Henning Löwe

Interactive comment on “Relating optical and microwave grain metrics of snow: The relevance of grain shape”, by Q. Krol and H. Löwe.

General comments:

This paper addresses the relation between the grain metrics commonly used to model snow optical and microwave properties. At first order, snow microwave properties are governed by the exponential correlation length ξ while snow optical properties firstly depend on snow specific surface area (SSA). However, at second order snow grain shape also affects snow radiative properties. From this statement, statistical relations are derived that make the link between snow microstructure characteristics (curvatures) and snow physical properties. The relation between ξ and SSA is thus improved compared to previous empirical relations, by adding a contribution of snow grain shape. The general theoretical framework of Malinka (2014) is then used to show that snow optical properties depend on the moments of the chord length distribution. Based on this framework, another statistical relation is derived to express the second moment of the chord length distribution in terms of microstructure length scales. From this, a statistical relation between ξ and the first two moments of the chord distribution is derived. This suggests that shape parameters derived from optical measurements could be used as inputs for snow microwave modeling. This point is supported by comparing the values of the optical shape parameter B deduced from Malinka (2014) theory to values determined experimentally.

The paper is overall well written and pleasant to read, the objectives are well defined at the end of the introduction. The theoretical background is nicely presented and clearly outlines the problem. The approach is original and takes advantage of recent works in snow optics. It also applies the statistical properties of general random heterogeneous materials to the case of snow, thus linking rather theoretical studies and practical cases as illustrated by the use of µCT images of snow samples. The authors stress the need for a unified definition of grain shape and propose mean curvatures as such definition. They show that both microwave and optical properties can be expressed in terms of SSA and mean curvatures. Their approach is supported by the analysis of a large set of µCT images. They also provide valuable physical insight on the representation of snow microstructure as a particulate or heterogeneous medium. For these reasons, I recommend this paper be published in The Cryosphere. However, a number of critical points should be addressed before publication, related in particular to the fundamental assumptions underlying the presented theoretical framework.

Specific comments:

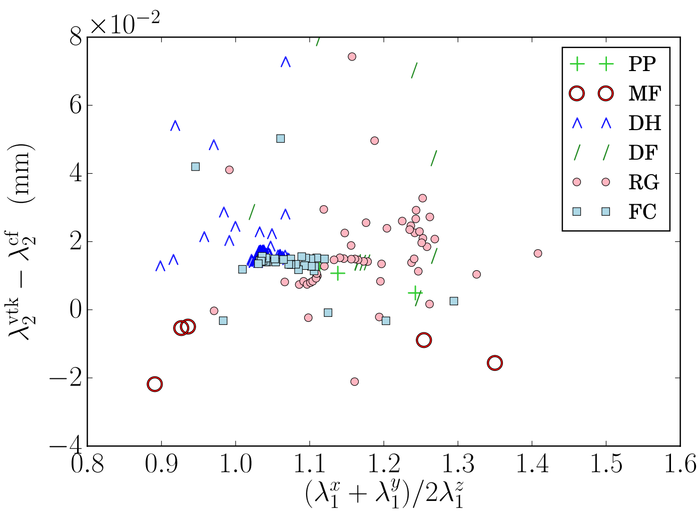
The theoretical framework presented in this paper strongly relies on critical assumptions that are not sufficiently discussed, although several important results largely depend on them.

1) Throughout the text, snow is considered isotropic and the derivations significantly rely on this critical assumption. Although this assumption is clearly stated, several details are lacking to convince the reader that the results remain reliable. First, more details on the investigated snow samples should be provided. So far only 3 lines (section 3.1) present these critical

elements of the study, which is not enough. Do these samples consist of sifted snow, natural snow samples taken in the field without perturbing the microstructure, snow samples resulting from metamorphism experiences in the laboratory...? It is clear that depending on the origin of the samples, the isotropic hypothesis is more or less acceptable. For instance depth hoar is known to be highly anisotropic and can hardly be investigated under this hypothesis. The authors should consider removing highly anisotropic snow samples if they do not fit in the theoretical background.
At the same time, the authors do have the necessary material to further discuss the isotropic hypothesis because the parameters are obtained from averages over the 3 directions x, y and z. Giving a hint of the actual anisotropy from the analysis of these 1-D parameters might help the interpretation of the data and estimate the associated uncertainties.

Reply:
We probably did not sufficiently elaborate on that point. To begin with, it is important to note that, strictly speaking, our analysis does not *assume* isotropy. We rather employ (wherever necessary) orientational averaging to reduce the information that is eventually used for the analysis. The geometrical interpretation of the involved quantities does not rely on isotropy. As an example, the relation between the slope of the correlation function via λ_1 and the surface area hold also (rigorously) for arbitrary, anisotropic systems, *after* orientational averaging (Berryman.1987). The same is likely true also for λ_2, namely that the orientational average of the third derivative of the correlation function of an anisotropic system is related to interfacial curvatures in the suggested way. We did not find a mathematical proof of the latter statement in literature, but our comparison of λ_2 (obtained from the correlation function, orientationally averaged) with λ_2 (obtained from direct computation of the interfacial curvatures) strongly suggests its validity. As an additional confirmation, we checked (plot below) that the remaining scatter is not caused by anisotropy, by plotting the residuals between the estimate λ_2^{vtk} (where anisotropy does not play a role) and λ_2^{cf}, which is not correlated with the anisotropy (R^2=.026). Accordingly, we also use the other length scales in the meaning of orientational averages, of arbitrary anisotropic systems. For the exponential correlation length this has been done similarly before. That said, none of the samples must be discarded.
Criticality of this procedure (not assumption) can only be revealed by measurements that will decide about the relevance of these orientationally averaged length scales for a measurement of anisotropic nature.

Changes to the manuscript: We add a part to the Discussion that discusses the anisotropy and retrieval of the parameters, however without showing this plot.



2) In this study, the successive chords in snow are assumed independent, which is a strong assumption not really defended by the authors. This same assumption was used by Malinka (2014) who considered a random medium, whose optical properties where then derived.

However, this author clearly states in his conclusion that: “The requirement of stochasticity is mandatory: the facets orientation and the ray path length inside solid or voids must be independent variables. [...] The question of applicability of the model to any particular medium should be considered separately based on compliance with the experimental data.” Practically, one might expect light rays to be trapped in snow grains or selectively focused in preferential location, which would result in different chords having different realization probabilities.

A critical consequence of the random distribution hypothesis is that at low ice absorption, the optical properties of this random medium do not depend on the shape parameter (see e.g. eq. (25) of Malinka (2014) from which B can easily be derived). This is somehow contradictory with the definition of grain shape, which is expected to impact snow optical properties in the standard particular representation.

An alternative approach could be to validate this random medium assumption by comparing the values of B retrieved from Malinka (2014) to those determined by Libois et al. (2014), which are very similar. Once the random medium hypothesis is somehow validated, then the shape parameter only impact optical properties at more absorbing wavelengths. An important corollary of this would be that only optical measurements at relatively absorbing wavelengths would contain information about snow grain shape.

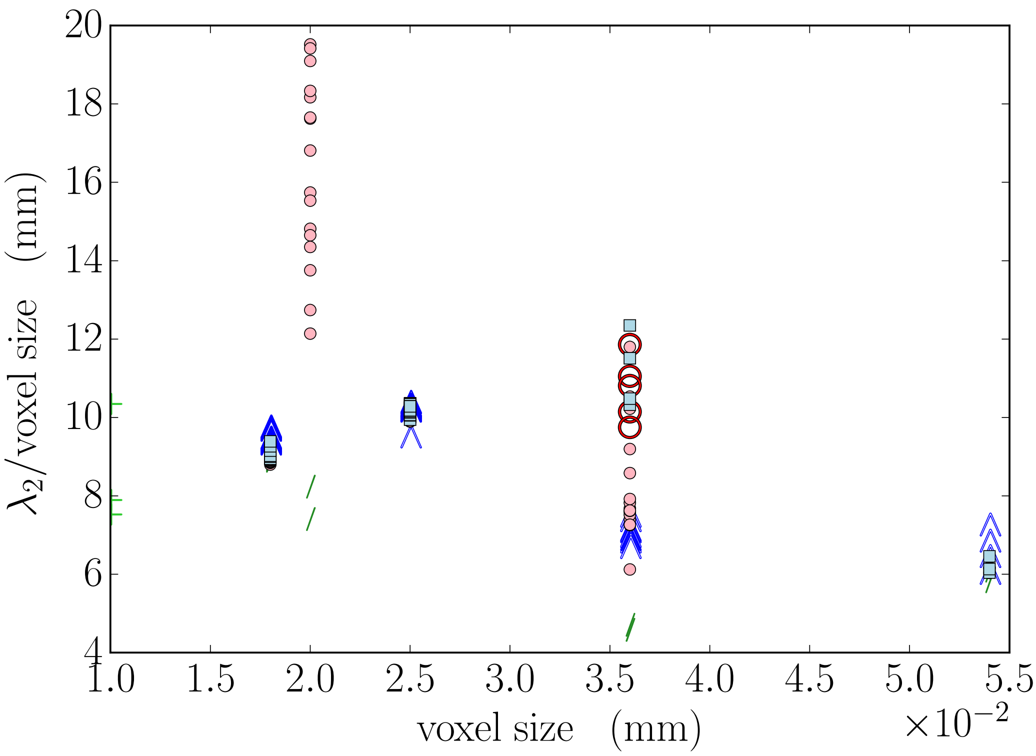
Reply:

We agree that for this step of deriving the shape parameter B from Libois 2013 by using Malinka 2014 involves a particular assumption about the independence of chords and adjacent surface normal orientations (note that our analysis of the statistical links between the length scales is however not affected by this) This issue was also brought up by the other reviewer, however rather pointing out the assumption of low absorption underlying Libois 2013 (which in contrast does not affect Malinka 2014). We are thus faced with the situation of linking two models/expressions that are based on two different, disjunct assumptions. That said, it is not entirely correct of using the closeness of the values found here to the values from Libois 2014 to confirm that the assumption of independent chords is not very restrictive. This aspect is now explained in more detail when deriving and discussing this connection. In the end (to produce Fig8) we evaluate B in the limit of low absorption (to cope with Libois). It is important to note that the assumption of independent chords (used in (Roberts and Torquato) already mentioned now in the paper) is slightly different from the assumption used by Malinka 2014. This will be also made clear.

Changes to the manuscript: The derivation of B is extended g^G, and the assumptions are discussed.

3) When it comes to the analysis of μCT images, the question of voxel size (ie resolution) is not enough discussed. In fact, the resolution varies from a set of measurements to another and is generally not that small compared to snow size metrics. This probably has an effect on the derived results and might explain why different subsets of points appear on several Figures (e.g. 2 bottom left and 4a). The smoothing parameter is discussed in sufficient details but resolution is probably an issue as critical.

Reply: We agree that the possible impact of the resolution could influence the results if the obtained quantities of interest are within a similar range. In general, the choice of resolution for CT images is made in accordance with the structure, such that the sample/resolution is statistically representative for the main quantities of interest (density and specific surface area). To assess the reliability of the obtained results we have compared them to the alternative VTK based method, for which we find very similar results. If the values for s are compared to the values that are obtained by the vendor software, we also see a good agreement with the VTK based method. To further confirm that the main quantity λ_2 is not systematically affected by image resolution we have plotted below the ratios of λ_2/voxelsize as a function of voxelsize, which are on average 9.8 with a standard deviation of 2.6. Only two samples have ratios 4.5 and the rest is 6.0 and higher. The correlation with the voxel size is R^2=-.20, but overall there is no systematic trend in λ_2/voxelsize for lower resolution (which would indicate a worse representation of the characteristic scales).



Changes to the manuscript:
We added a sentence on the spatial resolution of the data sets, its general importance and added the values for the characteristic ratios λ_2/voxelsize (the plot is however not included)

4) Although snow optical properties equally depend on the parameters B and g, the paper is mostly focused on B. The analysis presented for B can very easily be extended to g. This would be more exhaustive because all parameters relevant to snow optics would be tackled, as all parameters (actually only ξ) needed for snow microwave modelling are.

Reply: We agree that this extension to g (or g^G) is worthwhile for a comparison to Libois.2013. We replaced figure 8 by a plot of 1-g^G versus B (similar to libois.2013).

Changes to the manuscript: Table 1 is extended and Fig.8 is replaced by the a plot of B versus 1-g^G

5) The manuscript would benefit from a slight reorganisation of some parts because redundancy is found at several points and excessive details sometimes pollute the paper. Some elements are given too early (e.g. details about the Euler characteristic that should probably not be mentioned before the discussion section), some others should be provided in a different order (more details are provided along the technical comments). Also sections 3.3 and 3.4 could probably be merged.

Reply: We agree, this is also in accordance with a suggestion of the editor. As suggested, the definition of the Euler characteristic in the theory section is left out left out, since it is not explicitly required. The Discussion section is restructured. It discusses first the methodology, including resolution, anisotropy, and the geometrical interpretation of λ_1 and λ_2. Afterwards, that the statistical models are discussed. We finalize it by discussion grain shape, including the connection to (Libois.2013,2014) and (Malinka.2014).

Changes to the manuscript: As indicated above.

6) The authors make their best to infer the shape of the statistical relations from theoretical backgrounds. However, this often adds noise to the paper because 1) the underlying assumptions are often very restrictive and not applicable to snow (dilute medium, random medium, use of Taylor expansion at 0 for estimating functions at infinity...) and 2) these statistical relations are eventually revisited by adding terms. I think there is no problem assuming a certain type of relation, and then testing it with the available data. For sure, the type of relation can be suggested by a rapid analysis of existing formulae, but there is no need trying to justify it too much. In this context, I would suggest to remove the unnecessary calculations and reformulate the section around Eqs. (14) and (15). For instance the authors could say that they show the validity of Eq. (14) from images, even though initially this relation is only valid to restricted cases. All the attempts to justify this equation are unnecessary

   Reply: We agree. This is also in accordance with the other reviewer. These points are left for the discussion.

   Changes to the manuscript: The motivation for eq.15 is removed and this section is reformulated.

7) The authors should give a consistent name to all important quantities ξ, λ_1 , λ_2, μ_1, μ_2 and keep those names all along the manuscript. For instance, exponential correlation length and correlation length are sometimes used alternatively without a clear distinction. Porod length, optical diameter and curvature length are used sporadically as well.

   Reply: This was basically an attempt to stick to the names previously used in literature. But we agree, naming is now consistent and less ambiguous: λ_1 is named the Porod length, λ_2 is named the curvature length, the name for ξ, the exponential correlation length, remains. For μ_1 and μ_2 we stay with the first and second moment of the chord length distribution.

   Changes to the manuscript: The naming is made consistent throughout the manuscript.

8) At the light of the comments above, it will probably be necessary to rewrite the last section of the discussion (5.4).

   Reply: We agree, see comment 5).

   Changes to the manuscript: The discussion rewritten, taking all comments from both referees into account

Technical comments:

Could "snow grain size" be used instead of "grain metrics of snow"? Alternative suggestions (these are only suggestions):
- "Relating optical and microwave snow grain size: The importance/relevance of using/considering grain shape"
- "Accounting for snow grain shape to improve the relation between optical and microwave snow grain size"
We agree (maybe) to be discussed.

<u>Abstract:</u>

p.1 l.1: rephrase to better compare the roles SSA and exponential correlation length play in determining snow optical and microwave properties. Either from the physical point of view: "microwave emissivity/properties mostly depend(s) on the exponential correlation length". Or from the modelling point of view : "the exponential correlation length is the relevant quantity in most snow microwave models" or "the exponential correlation length is used to simulate snow microwave properties"
Reply: We agree.
Changes: The sentence is changed to "the exponential correlation length is the relevant quantity in most snow microwave models".

p.1 l.3: a microwave model is not "forced" by optical measurements, it uses quantities derived from optical measurements (e.g. SSA) as inputs. Forcing more generally refers to something external to the system (e.g. boundary conditions). This is correctly said p.2 l.9.
Reply: We agree.
Changes: "To facilitate forcing of microwave models by optical measurements" is replaced by "to derive input quantities of microwave models from optical measurements".

p.1. l.3: "the understanding of ξ" is vague. Simply say "To refine this relation between...]"
Reply: We agree.
Changes: the sentence is adjusted to "To refine the relation between…"

p.1 l.5: it is a statistical relation more than a prediction
Reply: We agree.
Changes: "Prediction" replaced by "relation".

p.1 l.8-9 : maybe remove this sentence because it does not provide additional information about the results. Also, it is somehow questionable in terms of applicability within the present theoretical framework. Keep it for the body of the manuscript.
Reply: We agree.
Changes: Deleted**.**

p.1 l.10 : B is called the absorption enhancement parameter. Consider doing the same calculations with g.
Reply: We agree.
Changes: The parameter g, and therefore g^G, can be directly inferred from (Malinka.2014). This is added to the analysis and abstract.

p1. l.10 : the last sentence of the abstract is not clear. Maybe say "Our results suggest that optically derived shape parameters can be used to refine the estimation of ξ".
Reply: We agree.
Changes: Last sentence changed to say "Our results suggest that optically derived shape parameters can be used to refine the estimation of ξ".

<u>Introduction</u>

p.1 l.16-19 : maybe invert the order of the two sentences to keep chronological order
Reply: We agree.
Changes: The sentences are inverted.

p.2 l.4 : "with the MEMLS model" instead of "is used"
Reply: We agree.
Changes: Adjusted accordingly.

p.2 l.14 : "though less significant..." is risky because the impact can actually be significant (errors up to 50%) for BRDF or light penetration simulations for instance.
Reply: We agree.
Changes: Changed.

p.2 l.16 : reference to Picard et al. (2009) might be relevant
Reply: We agree.
Changes: Reference is included.

p.2 l.17 : in this study the absorption enhancement parameter B and asymmetry factor g (name these factors) are equally important, except that only B can be estimated from optical measurements. Note that Libois et al. (2014) experimentally determined the parameter B for a variety of natural snow samples.
Reply: Thanks for pointing this out; we have not been aware of the paper.
Changes: Sentence on the measurement of B is added, including the citation. The discussion of B comes back to this point.

p.3 l.1 why "systematically?"
Reply: No specific reason.
Changes: Systematically is deleted.

p.3 l.12 : not clear what "images" you're talking about
Reply: We agree.
Changes: "images" is replaced by "µCT images".

p.3 l.15-17 : maybe keep those last 2 sentences for the discussion and mention it more shortly at this stage because this is hard to understand without the whole paper in mind.
Reply: We agree.
Changes: Rephrased

Theoretical Background

p.3 l.21-22 : very redundant with p.1 l. 20-21.
Reply: We agree.
Changes: The sentence has been reformulated.

p.4 l.5 : why "in contrast"? Is the exponential approximation only valid for large r values?
Reply: We agree. The exponential approximation is of course based on a fit for *all* r.
Changes: We removed "In contrast" from the sentence.

p.4 l.14: use m2 kg-1 instead
Reply: We agree.
Changes: Adjusted accordingly.

p.4 l.24-28 : consider mentioning the topological dimension of the mean Gaussian curvature only in the discussion, because at this stage the reader does not understand the point.
Reply: We agree.
Changes: Removed and included in the discussion.

p.4 l.26: the mathematical notation is not clear. Maybe use dS or dA to explicitly state that this is an average on the surfaces? This integration element could also be moved after the integrand.
Reply: We agree. The reference to the Euler characteristic is however moved to the discussion.
Changes: Adjusted accordingly.

p.4 l.27: that the local. Why is local in parenthesis?
Reply: Local refers to the fact that the determination of this part of the correlation function is an average over nearest (or next nearest) neighbours (in the voxel images) which is commonly referred to as "local". This is contrasted non-local (i.e. long range) effect.
Changes: The sentence is moved to the discussion, and local is removed to avoid confusion.

p.6 l.10: detail why z is actually small and mention in which conditions this theoretical framework is valid. This in in fact detailed below, but inverting the order might be helpful.
Reply: The text could indeed improve from reordering these sentences.
Changes: Reordered accordingly.

p.6 l.13 : to the theory of
Reply: We agree.
Changes: ‘the’ is inserted.

p.6 l.14 : it's 4π rather than 2π.
Reply: We agree.
Changes: Changed accordingly.

p.6 l.20: state here that the following sections investigate this issue and try to find a geometrical meaning of this second moment.
Reply: We agree.
Changes: A sentence is inserted.

p.7 l.2 : would it be useful to briefly define the surface-void correlation function? Otherwise
Reply: We won’t go into the precise definition of the surface-void correlation function since it does not affect the understanding of the method. It seems however justified to mention it here since this part indicates the required effort to improve the relation between the two point correlation function and the chord length distribution to be valid not only for dilute systems (comment from the other reviewer).
Changes: No

p.7 l.4 : please clarify the meaning of “this is not a practical limitation”
Reply: This question is related to the more fundamental question about the validity of independent chords from point 2.
Changes: see point 2.

p.7 l.1-7: since eventually the relation of Roberts and Torquato (1999) is not used, this part adds noise to the paper. Consider removing it (or mention it more concisely) if indeed it is not used.
Reply: We agree that we did not exploit this reference extensively. It is however crucial to comment on the assumption of the independence of consecutive chords.
Changes: The sentence is reformulated and used for a slightly different purpose (addressing point 2).

p.7 l.12: not clear why you keep going while snow is clearly not a dilute medium. If the relation actually holds for snow (which seems to be the case as you show its consistency), state there that you demonstrate its validity for snow.
Reply: We agree. (see also point 6). This point has been left out here since we come back to it in the discussion.
Changes: The section is cleaned up accordingly.

p.7 l.15: it seems that integrating by parts result in a factor [dA(l)/dl]. Why is it equal to 0? True for the exponential case. Idem for p.7 l.18
Reply: The two-point correlation (and thus its derivative) must go to zero for random systems for large r. Only in the presence of long range order (e.g. objects placed on a regular lattice) correlations persist to infinity (periodicity)
Changes: None.

p.7 l.20 : the expansion is only valid for small r values, while here the integration goes much beyond.
Reply: This equation is removed in the new manuscript, and therefore not discussed here anymore.
Changes: Revision of page 7.

p.7 l.20-24 : This paragraph somehow adds noise to the flow of the paper. Would it be problematic to make it shorter and simply state that in Eq. (15) the integral is a function of λ 1 and $\lambda 2$ and must be of “length” dimension? I think this would not change the use of this equation later on (section 4.4). This approach would also allow the use of a constant term in the fit of Eq. (21) without further justification.
Reply: We agree. Thank you for this suggestion, which serves as the basis for the new formulation.
Changes: Revision of page 7.

Methods

p.8 l.4 : More details about the preparation of the samples should be provided, and the isotropy of the prepared samples should be discussed. If for instance some samples obviously do not follow the

isotropy requirement (e.g. depth hoar) they should be removed from the analysis.
Reply: We agree that we could include more information on the samples that are used. Next to that, the isotropy (or rather absence of it) is mentioned. In the discussion session this is treated more extensively.
Changes: More information on the samples is given, and isotropy is shortly discussed.

p. 8 l.10 : the point regarding voxel size is very critical because the length scales are similar to voxel size, implying potential impact of voxelisation on the results. Can images at 18 and 50 µm be compared? See specific comment 3.
Reply: See answer to Comment 3.
Changes: We have discussed the effect of resolution in the methods and we come back to that in the discussion in more detail.

p.8 l.11 : before averaging, an evaluation of the anisotropy (or isotropy) should be given, because the whole theoretical framework is based on the isotropic hypothesis.
Reply: see answer on point 2
Changes: see comment 2.

p.8 l.15 : Figure 1b does not really illustrate the exponential regression
Reply: In fact the formula that is used to create this figure is an exponential function. The illustration is a graph representing the involved parameters.
Changes: Figure is adapted with an illustration of the retrieval of λ_1 and ξ.

p.8 l.23 : the meaning of "in view of shape" is not clear.
Reply: We agree.
Changes: This sentence is changed to: "To confirm the geometrical interpretation of λ_1^{cf} and λ_2^{cf} we use an alternative and independent method to estimate these parameters by measuring the surface area and the local interface curvatures with a VTK-based image analysis. In short… "

p.8 l.23-25 : state more clearly that the section aims at validating the Eqs (6) and (8) by computing the interfacial area and interfacial curvatures.
Reply: We agree.
Changes: see previous changes.

p.8 l.30 : could this smoothing parameter be slightly more detailed, because it seems critical in the following section. What's the typical range, what values were used in the past? For what kind of applications?
Reply: We agree. The smoothing parameter is a value for the number of times the Laplacian smoothing operation is applied. The smoothing has been discussed in (Krol.2016) and we adopted the same value for S here.
Changes: A short description of the filter is added.

p.9 l.4 : for S = 200, the interfacial area is larger, but the points seem also more spread, which is not discussed.
Reply: This is true. This is likely due to the fact that smoothing is filtering out small perturbations in the surface, reducing the area and increasing the values for λ_1. To which extend this happens is sample dependent, which causes the estimate for λ_1 to show a higher variance.
Changes: A sentence is added to clarify this.

p.9 l.6-11 : what is the objective of this section? Does it serve the paper? Should it be used to support the isotropic hypothesis?
Reply: We partly agree. We removed the figure but we kept this small paragraph to elaborate more on the surface representation and smoothing. The factor of 3/2 has been the origin of quite some confusion in the past, and we would like to take the opportunity to mention and hopefully clarify this point.
Changes: Figure is removed.

p.9 l. 16 : one should be with superscript "cf"
Reply: We agree.
Changes: adjusted.

Figure 2 (bottom left) : there seems to be 2 sets of points, one consisting of RG. Could this observation help interpreting the limitation of S = 50?
Reply: In fact there are as many 'groups' of data as there are time-series present, which naturally show a pseudo- continuous deviation from the curvature estimates. The deviations from the 1:1 line are caused by the overestimation of the curvatures by the remaining steps in the triangulation from the underlying voxel-based data, and is thus anti-correlated with the size of the structures and correlated with voxel size. In the end we chose a smoothing parameter that is, on average, acceptable for all involved samples.
Changes: A sentence is added to the discussion to clarify this apparent grouping of samples.

Figure 4a : there seems to be 2 sets of points. Do they correspond to similar subsets of µCT images? The same 2 sets are observed in Fig. 6a
Figures 4b and c : DH is clearly an outsider here. Is it relevant to keep it in this study?
Reply: As explained above, these two sets of points are correlated since they are part of a time series. We will emphasize this when the samples are introduced in section 3.1. The depth hoar samples that show a higher deviation in Fig 4b and 4c, do not have particularly higher anisotropy values than the other depth hoar samples that do not have high residuals.
Changes: The data is introduced in more detail as well as the fact that some of them are part of a time-series. The anisotropy is discussed in more detail in the reformulated discussion.

Results

p. 11 l.11 : one extra "and"
Reply: We agree.
Changes: 'The' is deleted.

p. 11 l.11 : is it consistent to have a R2
less (0.731<0.733) for the regression with an additional
parameter?
Reply: Yes it is, since fitting eq.(18) includes two extra parameters which, if done correctly, should be accounted for in an adjusted correlation coefficient. Since a_0 is negligible to the fit this does not show in R^2 but it is however penalized in the reduced correlation coefficient.
Changes: we included "adjusted correlation coefficient".

p.13 l.1 : the name of $\lambda 1$ should be consistent between titles of sections 4.1 and 4.2. In section 4.1, optical diameter is not mentioned except in the title.
Reply: We agree.
Changes: The subtitle is changed from "Relating exponential correlation length to optical diameter" to "Relating exponential correlation length to the Porod length".

p.13. l.7 : I don't really understand this justification and don't think this is necessary. I would proceed the other way round instead. The figure 4b could be discussed at the end of section 4.1 with the aim of understanding the remaining residuals. This would naturally lead to the regression Eq. (19).
Reply: We agree.
Changes: The order is reversed.

p.13 l.13 and 14: Eq. (14) instead of (16)
Reply: We agree.
Changes: Adjusted.

p.14 l.3 : Eq. (15) in stead of Eq. (14)
Reply: We agree.
Changes: Reference adjusted.

p.14 l.17 : here you try "heuristically" a regression, which is fine. This somehow contrasts with the previous regressions that were based on the derivation of equations. This could also be motivated by the form of Eq. (13) that includes the porosity factor. I think there is no problem assuming a relation,

and then testing its validity with measurements. This is sometimes easier to understand than long inexact derivations.
Reply: We agree. In this section we changed the motivation for the statistical models involved.
Changes: We reformulated this sentence to "To motivate a statistical model we start from eq.(15) and test different expressions for $f(\varphi,\lambda_1,\lambda_2)$. Since f has dimension length a natural first candidate would be.. ". l.8: The sentence "Although not predicted from Eq.20…" is removed.

p.14 l.12 : it is awkward to read that the benefit is small but to see the new regression, though. I would put it more positively: "The correlation coefficient ($R2=0.295$) is small but including λ2 in the analysis further improves the fit".
Reply: We agree.
Changes: adjusted

p.14 l.24-25 : this is sometimes disturbing to read "correlation length" at some point and "exponential correlation length" later on. Please remain consistent throughout the manuscript, with each quantity (ξ, λ1, λ2) having its dedicated and constant name. Consider using "exponential" for the first part of the sentence, and "correlation length scales or Porod length and curvature lengths (for instance)" for the second part, to make the link with Eqs. (19) and (23) more obvious.
Reply: See comment 7. To avoid confusion between the exponential correlation length and correlation length we stick to the term Porod length for λ_1.
Changes: Naming changed.

Figure 6 : remove "see". λ1 is not the optical diameter.
Reply: We agree.
Changes: Removed "optical diameter", changed to Porod length.

<u>Discussion</u>
p.16 l.2 : in complement to this discussion, this might be worth giving the sensitivity of Eq. (16) to the smoothing parameter, and possibly to the voxel size as well, if this makes sense.
Reply: The smoothing parameter only influences the VTK-based parameters. The voxel size has an impact on the estimates of λ_1, λ_2, μ_1 and μ_2 and will be discussed in more detail.
Changes: Voxel size is detailed in the discussion.

p.17 l.5 : remind what grain size is because a1 is the coefficient for λ1 (which is optical diameter or grain size?)
Reply: We agree.
Changes: We adapted this sentence to "As a first step we have analysed the statistical relation between exponential correlation length and the Porod length. The latter is referred to as simply "grain size" or correlation length in Mätzler(2002)".

p.17 l.6 : again depth hoar could be removed from the analysis if it does not satisfy the conditions of the theoretical framework.
Reply: As discussed under point 1. Accordingly, we will argue in favour of keeping these samples.
Changes: None.

p.17 l.7 : this is not clear what is also shown by those data. That the coefficient is larger for depth hoar?
Reply: The results from Mätzler(2002) also distinguish depth hoar $\xi=.8\lambda_1$ and other snow types $\xi=.6\lambda_1$.
Changes: The sentence is changed to "Mätzler's model predicts $a1 = 0.75$, which is an average of $a_1=.8$ for depth hoar and $a_1=.6$ for other snow types. Comparing this to our result, $a_1=.79$, this is consistent since we have many depth hoar samples in the data set, which indicates an even larger influence of snow type or grain shape."

p.17 l.21 : Eq. (7) instead of Eq. (1)
Reply: We agree.
Changes: adapted

p.17 l.32 : there were attempts

Reply: We agree.
Changes: adapted

p.18 l.5 : why is "independent" in italic. Idem for p.18 l.15 "if"
Reply: We agree that it is not necessary to stress the words 'independent' and 'if'.
Changes: Adapted.

p.18 l.5 : where does this K/3 come from? It is K/24 in Eq. (8)
Reply: Yes, K/3 must be compared to $H^{2.}$
Changes: We adapted Eq(8) to 1/8(H^2-K/3) to make this obvious.

p.18 l.12 : this point is interesting, but puzzling as well. Indeed, from an optical point of view, a polydispersion of spheres will have the same "shape" parameters as a monodispersion in the geometrical optics approximation (and for low ice absorption), because B and g primarily depend and the shape, not on the size. Hence polydispersion would affect curvatures, but not grain shape as defined from an optical point of view. Said differently, a polydispersion of spheres will have optical properties similar to a monodispersion with same SSA, but different microwave properties.
Reply: We agree.
Changes: None.

p.18 l.32 : for such a system?
Reply: Yes.
Changes: Changed.

p.19 l.10 : wavelengths (in a single word?)
Reply: We agree.
Changes: wave lengths -> wavelengths.

p.19 l.12 : the mentioned paper rather suggests that g for spheres is larger than g for snow, and that B for spheres is smaller than B for snow.
Reply: We agree. This is also consistent with the values we calculated for g and B shown now in Fig.7
Changes: Adapted.

p.19 l.12 : the superscript G for the g refers to "geometrical", that does not account for the diffraction contribution to scattering. This does not change the sentence but should remain consistent throughout the paper.
Reply: We will use consistently g^G and B.
Changes: notation adapted.

p.19 l.12 : it depends on shape rather than includes it
Reply: We agree.
Changes: include->depends

p.19 l.16 : it's 4π rather than 2π. By the way this quantity was already defined p.6. Then check the values for the following text and those shown in Table 1.
Reply: Checked
Changes: None.

Table 1:

Fraction of second to first rather than first to second order. Precise that mean and standard deviation are among all samples. Write 170 rather than 1.7 x 102.
The values suggest no influence of shape at 0.9µm, which is consistent with the remark p.18 l.12.

Note that eq. (5) of Malinka (2014) shows that at weakly absorbing wavelengths, B only depends on the real part of the refractive index.

This latter point should be further discussed to explore the validity of the random medium assumption used by Malinka (2014). In fact, this framework suggests that as long as the structure is random, shape has no impact on optical properties. This is contradictory to the fact that in the particulate representation of snow, different grain shapes result in different optical properties, even at low ice absorptions

Reply:
We adapted the notation and description in Table 1.

We agree that Malinka involves a particular assumption on the independence of chords and adjacent surface normal orientations. This apparently leads to $B=n^2$ in the limit of very small alpha. This is now explicitly shown in the appendix. We also calculated there the next order correction in alpha that shows a slight dependence of B on shape if the latter would be defined only via moments of the chord length distribution. Accordingly, for visible wavelengths and corresponding alpha, no shape dependence of B would be predicted from A4, which is indeed not what is observed in nature. Thus it might be the case that, by using this independence assumption, some influence of shape on B is lost, in particular for for very low alpha (visible).

Changes: We included these points in the Discussion.

p.20 l.6 : the authors decide to emphasize the parameter B, but in fact eq. (60) of malinka (2014) can also be used to express g in terms of λ1 and λ2. This should be done to complete the analysis.
Reply: We agree. The analysis is extended to g
Changes: New figure with a plot of g versus B.

p.20 l.7 : why is the parameter B shown in terms of this ratio? Is there supposed to be a visual correlation in Fig. 8? Why is the regression with respect to this particular ratio?
Reply: This was done because eq.A4 is a function of p(α), and the ratio determines the relative importance of first and second order terms. However this figure is now replaced by a plot of g versus B. But the ratio can be also used as a simple proxy to assess the deviation of the snow chord length distribution from an exponential one (see comment 6 in the other review) Values are therefore given in the text.
Changes: Figure changed.

p.20 l.9 : Libois et al. (2014) experimentally determined the parameter B for a large set of snow samples and suggest B equals 1.6 ± 0.2. This comparison completes that with Libois et al. (2013). Note again that the range obtained in Fig. 8 results from the impact of shape at 1.3µm. This range can hardly be compared to that obtained by Libois et al.(2013,2014) obtained at visible wavelengths. The absolute values can on the contrary be compared.
Reply: We will emphasize the difference in the wavelength and discuss that in the weakly absorbing limit B is only depending on the real part of the refractive index. We will also point out that the apparent increased variation of B observed for visual wavelengths, may be due to the shadowing effect/density as discussed in (Libois et al (2014).
Changes:

p.20 l.9-12 : these sentences are not clear, and reference to Haussener et al. (2012) is very fuzzy, in particular the “remaining discrepancies”.
Reply: we agree.
Changes: reference removed

p.20 l.15 : involved
Reply: We agree.
Changes: adapted

p.20 l.20 : this is the very critical assumption that should be further discussed
Reply: We agree. This assumption is indeed critical, but rather difficult to investigate. As explained above, we can only discuss this in reference to (Roberts and Torquato) who established an improved relation between the chord length distributions and the correlation functions. Their improved relation is still based on the assumption of independent chords. They tested this for level-cut Gaussian random fields, where successive chords are not independent from a rigorous perspective. The results however agree reasonably well, which is at least an indicator that this assumption is not so critical for this

aspect. As mentioned before, this independence assumption is however still slightly different from the independence assumption used by Malinka 2014.
Changes: This point is emphasized in the discussion which has been restructured.

p.21 l.l.1-16 : This part shows is partly redundant with previous parts of the text. This could be shortened.
Reply: This part of the text is replaced and rewritten to avoid redundancy.
Changes: Discussion is restructured and rewritten.

p.21 l.11 : why is this work mentioned here and not before? Could this help to establish the semiheuristical relations displayed all along the manuscript?
Reply: This relation is introduced in the discussion since it only explains that the slope in the origin of the chord length distribution is related to λ_2. While this shows yet another connection between chord lengths and the curvature lengths, worth mentioning, we were not able to put this on more general grounds which could be exploited earlier.
Changes: None.

p.21 l.12-14 : Why is the variance of the chord length distribution mentioned here for the first time?
Reply: Because it emerges only here in this argument to connects mu2 to lambda_12
Changes: In the reformulated discussion the variance of the chord length distribution is left out.

p.21. l.19 : remove parenthesis in reference
Reply: We agree.
Changes: removed

Conclusions

p.21 l.29 : extra "we"
Reply: Yes.
Changes: Changed.

p.21 l.29 : consider adding (λ2) after size metric
Reply: We agree.
Changes: added

p.22 l.9 : the meaning of "when compared to" is not clear
Reply: we agree.
Changes: rephrased.

p.22 l.9 : Maybe say : "The consistency between B values derived from the chord length distribution and those determined from optical measurements suggests such an approach is indeed possible".
Reply: We agree,
Changes: Changed accordingly.

Appendix

p.22 l.28 : no parentheses for the references
Reply: We agree.
Changes: parentheses removed

p.23 l.8 : by the Swiss...
Reply: we agree.
Changes: The typo is removed.

References by the referee:

Haussener, S., Gergely, M., Schneebeli, M., & Steinfeld, A. (2012). Determination of the macroscopic optical properties of snow based on exact morphology and direct pore- level heat transfer modeling.

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Picard, G., Arnaud, L., Domine, F., & Fily, M. (2009). Determining snow specific surface area from near-infrared reflectance measurements: Numerical study of the influence of grain shape. Cold Regions Science and Technology, 56(1), 10-17.

References by the author:

Berryman, James G. "*Relationship between specific surface area and spatial correlation functions for anisotropic porous media*." Journal of mathematical physics 28.1 (1987): 244-245.

Relating optical and microwave grain metrics of snow: The relevance of grain shape

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Abstract. Grain shape is commonly perceived as a characteristic of snow beyond the optical diameter (or specific surface area) which influences the physical properties. In this study we use tomography images of snow to investigate two objectively defined metrics of grain shape which naturally extend the characterization of snow in terms of the optical diameter. One is the curvature-length, λ_2, related to the third order term in the expansion of the correlation function and the other is the second moment of the chord length distributions, μ_2. From the first, we make contact to microwave modeling via the exponential correlation length ξ and show that grain shape explains the remaining scatter when ξ is statistically related to the optical diameter. From the second, we make contact to a geometrical optics framework via the absorption enhancement parameter B and asymmetry factor g^{G}. We establish various statistical relations between all size metrics obtained from correlation functions and chord length distributions. Overall our results suggest that the definition of grain shape via λ_2 or μ_2 is virtually equivalent. Both capture aspects of size dispersity in snow and constitute an intersection between microstructure characterization for optical or microwave modeling.

1 Introduction

Linking physical properties ~~and microstructure of snow is a fundamental task of snow science. The~~ of snow to the microstructure always requires to identify appropriate metrics of grain size. In this regard, the two-point correlation function ~~of snow~~ has become a key quantity ~~in this respect~~ for the prediction of various properties such as thermal conductivity, permeability and electromagnetic properties of snow (Wiesmann and Mätzler, 1999; Löwe et al., 2013; Calonne et al., 2014b; Löwe and Picard, 2015). The ~~recent gain in interest of correlation functions is mainly driven by available data from micro-computed tomography (μCT), from which the correlation function can be conveniently estimated. The~~ correlation function carries, in essence, information about a distribution of relevant sizes in the microstructure. For microwave applications, the analysis of correlation functions ~~for microwave application dates back to the pre-~~ was already used in the era before micro-computed tomography (μCT~~era~~), where thin section data and stereology were ~~used~~ employed to obtain the required information (Vallese and Kong, 1981; Zurk et al., 1997; Mätzler and Wiesmann, 1999).

~~The~~ The recently gained interest in correlation functions is mainly driven by available data from μCT, from which the correlation function can be conveniently estimated. The relevance of the two-point correlation function for microwave modeling originates from the connection between its Fourier transform and the scattering phase function in the Born approximation for small scatterers (Mätzler, 1998; Ding et al., 2010; Löwe and Picard, 2015), or the connection to the effective dielectric tensor via depolarization factors (Leinss et al., 2015). ~~A common~~

A common practical way to characterize the correlation function is a fit to an exponential, such that the fit parameter, the so called exponential correlation length ξ, can be used to model the decay of ~~structural~~ microstructural correlations in snow by a single size parameter. This approach dates back to Debye et al. (1957) in the context of small angle scattering of heterogeneous materials. However the characterization of snow ~~in terms of a single size metric~~ by a single length ξ is only an approximation since the ~~occurence~~ occurrence of multiple length scales (Löwe et al., 2011) are known to play a role~~in~~ , in particular to characterize anisotropy (Löwe et al., 2013; Calonne et al., 2014b). Despite ~~these fundamental caveats, the correlation length~~ this caveat, ξ still constitutes the main microstructural parameter for microwave modeling of snow (Proksch et al., 2015a; Pan et al., 2016) ~~if~~ when the Microwave Emission Model of layered snowpacks (Wiesmann et al., 1998) is used. ~~However, direct measurements of~~ ~~ξ~~~~, besides~~ ~~μ~~~~CT, do not exist and the~~

The exponential correlation length is often ~~statistically~~ inferred from measurements of the optical equivalent diameter d_{opt} or~~of~~ , equivalently, from the specific surface area (SSA). This link was established statistically (Mätzler, 2002) leading to the empirical relation

$$\xi \approx 0.5 d_{\mathrm{opt}}(1-\phi), \tag{1}$$

where ϕ is the ice volume fraction. This relation facilitates ~~the use of the~~ using the measured optical diameter as the primary input for microwave modeling (Durand et al., 2008; Proksch et al., 2015b; Tan et al., 2015). ~~Despite this practical advantage, such a relation~~ However, this link between ξ and d_{opt} can only serve as a first approximation~~, since the~~ . The numerical prefactor in Eq. (1) seems to depend on snow type (Mätzler, 2002) ~~, causing~~ which causes a significant scatter in ~~the estimates. This has neither been investigated in detail nor traced back to additional shape metrics~~estimating correlation length from optical diameter. This poses the question which additional size metric captures variations in grain shape and explains the scatter.

A similar issue of ~~shape, though less significant in order of magnitude,~~ grain shape emerges in the context of optical measurements. Optical properties (e.g. reflectance) can be largely predicted from the optical diameter or SSA (Kokhanovsky and Zege, 2004). The remaining scatter is ~~small but commonly also attributed to grain shape~~ commonly attributed to shape which influences the absorption enhancement parameter B and the asymmetry factor g^{G} (Picard et al., 2009) . The influence of ~~shape on~~ grain shape on B for light penetration was recently ~~quantified by Libois et al. (2013) in terms of a shape factor~~ addressed and measured by Libois et al. (2013, 2014) . Also in this case it remains the question which additional size metric of the microstructure can be used to capture variations in grain shape and measured scatter in B~~, which originates from Kokhanovsky and Zege (2004) . A systematic framework that principally allows to analyze this issue for geometrical optics was recently put forward by Malinka (2014) who derived closed-form expressions for the averaged optical properties. The relevant microstructural quantity is the chord length distribution (Torquato, 2002) or, more precisely, its Laplace transform. Thereby, the microstructural metrics used by Malinka (2014) , is not limited to a particular model microstructure (e. g, spheres) but can be applied to generic two-phase media which implicitly incorporates shape.~~ .

The two examples from microwave or optical modeling above reflect the known fact that the optical diameter as a single metric of grain size is not sufficient to characterize the microstructure for many physical properties. It is thus necessary to account for additional grain size metrics which implement the idea of grain shape. A key requirement for potential, new shape metrics is a well-defined geometrical meaning~~of the quantity. Presently, the exponential correlation length is essentially a statistical object which is still difficult to interpret beyond the empirical correlation in Eq. . This hinders the development of evolution equations in snowpack models, and the development of alternative, portable measurement techniques to estimate new parameters in the field for validation campaigns.~~ . Present snowpack models (Vionnet et al., 2012; Lehning et al., 2002) contain empirical shape descriptors such as sphericity (Brun et al., 1992). An objective definition of these quantities for arbitrary two-phase materials is, however, not possible. New shape metrics should thus ideally seek to replace empirical ~~microstructure~~ parameters by an objective, measurable and geometrically comprehensible ~~metric of the microstructure. An appealing candidate is a curvatures based metric, because i) curvatures~~ metrics.

One appealing route to define shape is via curvatures of the ice-air interface because curvatures i) have already been used to comprehend snow metamorphism via mean and Gaussian curvatures (Brzoska et al., 2008; Schleef et al., 2014; Calonne et al., 2014a) ii) ~~curvatures are natural~~ are natural quantities to assess shape via deviations from a sphere, very close to the ~~original idea of sphericity (Brun et al., 1992)~~ definition of sphericity in Lesaffre et al. (1998) and iii) ~~curvatures also~~ naturally emerge as higher order terms in the expansion of the correlation function (Torquato, 2002)~~, which closes the circle with the microwave context~~. The latter fact can be used in turn to assess variations of the microwave parameter (ξ) from μCT images which links back to the aforementioned microwave modeling problem.

Another appealing route to define shape is via chord length distributions because they i) naturally implement the idea of size dispersity and ii) have been recently put forward by Malinka (2014) to derive closed-form expressions for the averaged optical properties of a porous medium. Again, the latter fact can in turn be used to assess variations in the optical parameters (g^{G}, B) from μCT images which links back to the aforementioned optical modeling problem.

The motivation of the present paper is ~~three-fold~~to investigate and interconnect these two routes of objectively defining grain shape. First, we will ~~systematically assess the curvature term~~ assess the curvature-length in the expansion of the correlation function~~as a potential shape parameter~~. We will be guided by the question if and how the well-known statistical relation Eq. (1) between the exponential correlation length and the optical diameter can be improved by incorporating curvatures. Second, we will characterize the microstructure in terms of chord length distributions in order to make contact to aspects of shape in snow optics. ~~Third, we motivate~~ An interconnection between the two routes can be established by an approximate relation between the correlation function and the chord length distribution that was originally suggested in the context of small angle scattering (Méring and Tchoubar, 1968). ~~The relation suggests various connections between~~ By means of this approximate relation we establish various statistical links between all involved size metrics, the moments of the chord length distributions, optical diameter, surface areas, curvatures and the exponential correlation length. The ~~statistical analysis of these metric inter-relations leads to the announced~~ established links imply a microstructural connection between geometrical optics and microwave scattering ~~in the Born approximation, and an expression for the optical shapefactor B~~via size dispersity, which constitutes one aspect of grain shape.

The paper is organized as follows. In Section 2 we present the theoretical background for the correlation function, the chord length distribution, the ~~relation~~ connection between both quantities and the governing length scales. In Section 3 we provide a summary of the μCT image analysis methods. To provide confidence of the interpretation of the curvature metrics derived from the correlation function, we present an independent validation of these quantities via the triangulation of the ice-air interface. The results of the statistical models are presented in Section 4 and discussed in Section 5. ~~Due to the differences in lengthscales between optical and microwave metrics a connection between the two via shape may seem surprising. We therefore aim to illustrate this connection by discussing it in view of the appealing but limited picture of snow as a packing of irregularly shaped grains.~~

2 Theoretical background

2.1 Two-point correlation function and microwave metrics

The interaction of microwaves with snow are commonly interpreted as scattering at permittivity fluctuations in the microstructure ~~. This is reflected for example by the fact that in the Born approximation the scattering coefficient or the phase matrix is proportional to the Fourier transform of the~~ which can be described by the two-point correlation function ~~(Mätzler, 1998; Ding et al., 2010;~~ The correlation function can be derived from spatial distribution of ice and air that is characterized by the ice phase indicator function $\mathcal{I}(\boldsymbol{x})$, which is equal to 1 for a point $\boldsymbol{x}$ in ice and 0 for $\boldsymbol{x}$ in air. From that, a covariance function can be defined which is often referred to as the correlation function

$$C(\boldsymbol{r}) = \overline{\mathcal{I}(\boldsymbol{x}+\boldsymbol{r})\mathcal{I}(\boldsymbol{x})} - \phi^2. \tag{2}$$

In the following we disregard anisotropy by stating that $C(r)$ only depends on the magnitude of $r = |\boldsymbol{r}|$. To interpret snow with this approach, an average over different coordinate directions must be carried out.

The value of the correlation function $C(0) = \phi(1-\phi)$ is simply related to the volume fractions of ice and air. Therefore, often only the normalized correlation function

$$A(r) = C(r)/C(0) \tag{3}$$

is used, (see Fig. 1b). Since $A(r)$ must decay from $A(0) = 1$ to zero for $r \to \infty$, the correlation function is often described by an exponential form

$$A(r) = \exp\left(-r/\xi\right), \tag{4}$$

in terms of a single length scale, the exponential correlation length ξ, which empirically characterizes the decay of $A(r)$.

~~In contrast, for~~ For small arguments r, also rigorous results for the decay of the correlation can be inferred since the expansion of $A(r)$ can be interpreted in terms of geometrical properties of the interface. According to Torquato (2002), the expansion for an isotropic medium reads

$$A(\boldsymbol{r}) = 1 - \frac{r}{\lambda_1}\left[1 - \frac{r^2}{\lambda_2^2} + \mathcal{O}(r^3)\right] \tag{5}$$

in terms of the length scales λ_1, λ_2. The first order term

$$\frac{1}{\lambda_1} = -\left.\frac{d}{dr}A(r)\right|_{r=0} = \frac{s}{4\phi(1-\phi)}, \tag{6}$$

is the slope of the correlation function at the origin and can be expressed in terms of ~~s which is~~ the interfacial area per unit volume s (Debye et al., 1957). The size metric λ_1 is one of the most fundamental lengths scales for a two-phase medium and commonly referred to as the ~~Porod length~~ *Porod length* in small angle scattering, or ~~simply correlation length in Mätzler (2002)~~ *correlation length* in Mätzler (2002) . We will adhere to Porod length here to clearly distinguish λ_1 from the exponential correlation length ξ. The metric λ_1 can be also related to the SSA, defined as the surface area per ice mass (~~m^2/kg~~ $m^2 kg^{-1}$), or in turn to the equivalent optical diameter d_{opt} of snow via

$$\lambda_1 = \frac{4\phi(1-\phi)}{s} = \frac{4(1-\phi)}{\rho_{\mathrm{i}}\,\mathrm{SSA}} = \frac{2(1-\phi)}{3}d_{\mathrm{opt}} \tag{7}$$

with ρ_{i} representing the density of ice. The last equality is obtained when the definition of $d_{\mathrm{opt}} = 6/\rho_i\mathrm{SSA}$ is inserted (see Mätzler (2002)).

For a two-phase material with a smooth interface, the second order term $\sim r^2$ is missing in the expansion Eq. (5) and the next non-zero term is the cubic one with a prefactor $1/\lambda_1\lambda_2^2$. Here the length scale λ_2 ~~also~~ has a geometric interpretation in terms of interfacial curvatures ~~, hereafter~~ and is therfore referred to as the curvature length hereafter. As originally shown by Frisch and Stillinger (1963), the following identity holds

$$\frac{1}{\lambda_2^2} = \lambda_1\left.\frac{d^3}{dr^3}A(r)\right|_{r=0} = \cancel{\frac{\overline{H^2}}{8}}\frac{1}{8}\left(\overline{H^2} - \cancel{\frac{\overline{K}}{24}}\frac{\overline{K}}{3}\right) \tag{8}$$

in terms average squared mean curvature $\overline{H^2}$ and the averaged Gaussian curvature $\overline{K}$. The quantity λ_2^{-2} ~~it also referred to as Eulerian~~ is proportional to the orientationally averaged normal curvature of an interface (Tomita, 1986). ~~The averaged Gaussian curvature $\overline{K}$ is related to a topological quantity of the ice-air interface. It can be related to the Euler characteristic χ via the Gauss–Bonnet theorem~~

$$\chi = \frac{1}{2\pi}\int d^2x K(x) = V s\overline{K},$$

~~with V representing the total volume. This is noteworthy insofar, as the (local) expansion of the correlation function at the origin contains a topological (i.e. a global) property of the interface.~~

2.2 Chord length distributions and optical metrics

In ~~contrast to the interaction with microwaves, snow optics is based on a different~~ snow optics the microstructural characterization within radiative transfer theory (Kokhanovsky and Zege, 2004) ~~, which commonly employs~~ commonly involves a single metric, the optical diameter. An interesting ~~extension~~ approach for geometrical optics in arbitrary two-phase media was recently put forward by Malinka (2014). Thereby, the microstructure is taken into account by the chord length distribution of medium which can be unambiguously defined for arbitrary two-phase random media (Torquato, 2002).

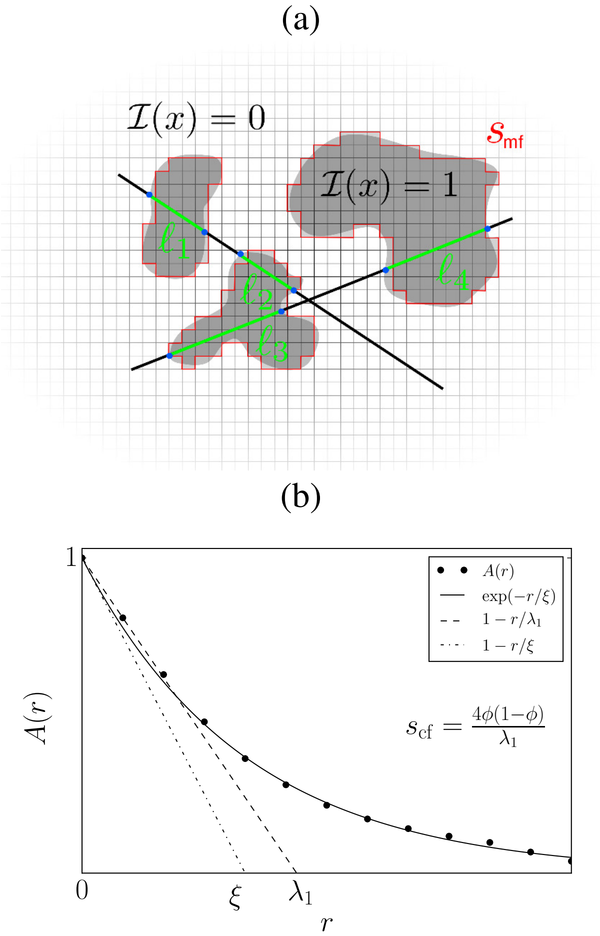


Figure 1. a) Illustration of the chord lengths obtained from an ice sample. The mean chord length is defined as the average length of the green line lengths. A stereological approach (Underwood, 1969) to calculate s is to count the number of blue dots per unit length. The estimation for s_{mf} is given by the red contour. b) Illustration of the correlation function $A(r)$ and the method obtaining an estimate for the Porod length λ_1 to get s_{cf} by fitting the slope at the origin, and the exponential correlation length ξ by fitting $A(r)$ to $\exp(-r/\xi)$ over a larger span.

Chord lengths in an isotropic medium ~~can be~~ are defined as the lengths of the intersections of random rays through the sample with the ice phase~~as shown~~, as illustrated in the schematic in Fig. 1a. The chord length distribution $p(\ell)$ of the ice phase denotes the probability (density) for finding a chord of length ℓ.

In contrast to the Born approximation for microwaves, where the microstructure enters as the Fourier transform of the correlation function, the theoretical approach Malinka (2014) relates the key optical quantities (absorption, phase function, asymmetry-factor) to the Laplace transform of the chord length distribution $p(\ell)$ which is denoted by

$$\widehat{p}(z) = \int_0^\infty d\ell \, p(\ell) \mathrm{e}^{-z\ell} \tag{9}$$

with Laplace variable z. ~~The Laplace transform is closely related to the moments~~ For small z, the Laplace transform can be approximated by the expansion

$$\widehat{p}(z) = 1 - \mu_1 z + \frac{\mu_2}{2} z^2 + \mathcal{O}(z^3), \tag{10}$$

where μ_i denotes the i−th moment of the chord length distribution, viz

$$\mu_{\cancel{n}i} = \int_0^\infty d\ell\, \ell^{\cancel{n}i} p(\ell). \tag{11}$$

~~since the expansion of the Laplace transform Eq. for small z can be written as~~

$$\cancel{\widehat{p}(z) = 1 - \mu_1 z + \frac{\mu_2}{2} z^2 + \mathcal{O}(z^3).}$$

~~This implies that the~~ Hence within the approach from (Malinka, 2014) , the optical response of snow can be systematically improved by successively including higher moments of the chord length distribution. According to ~~theory of~~ the theory Malinka (2014), the Laplace transform has to be evaluated ~~for~~ at $z = \alpha$, with the absorption coefficient ~~$\alpha = 2\pi\kappa/\lambda$~~ $\alpha = 4\pi\kappa/\lambda$. Here λ is the wavelength and κ the imaginary part of the refractive index of ice. It is generally sufficient (Malinka, 2014) to retain only a few terms in Eq. (10). It is straightforward to show (Underwood, 1969) that the first moment, i.e, the mean chord length μ_1 is given by

$$\mu_1 = \frac{4\phi}{s} = \frac{\lambda_1}{1-\phi} = \frac{2}{3} d_{\mathrm{opt}} \tag{12}$$

and thus related to the surface area per unit volume s from Eq. (6) ~~or one of its counterparts~~, or the optical diameter d_{opt} via Eq. (7). ~~Thus~~ Therefore, in lowest order, the Laplace transform Eq. (9) only contains the ~~optical radius~~ Porod length or specific surface area of snow. The next order correction involves the second moment μ_2 for which no geometric interpretation has been hitherto given for arbitrary two-phase random media.

~~The~~ For known chord length distribution ~~is closely related to stereological principles which have been widely used in the pre-μCT era (e.g., **??**), to estimate the density and the surface area per unit volume for snow and other crystalline materials. The connection to stereology is illustrated in Fig. 1a, where the well-known counting of the blue intersection points per unit length gives an estimate for the averaged interfacial area s~~, all optical quantities (phase function, anisotropy factor g^{G}, etc) can be directly computed from Malinka (2014) . To make contact to Libois et al. (2013) later and discuss our results for the chord lengths in light of shape, an expression of the absorption enhancement parameter B is required within the framework of Malinka (2014) which is done in the Appendix A. From these expressions we can asses the relative importance of the μ_2 correction to the optical diameter μ_1.

2.3 Connection between chord lengths and ~~correlation lengths~~ the Porod length and the curvature-length

Following the previous two sections, a link between optical and microwave metrics of snow thus requires to establish a link between correlation functions and chord length distributions. ~~This issue has been discussed by Roberts and Torquato (1999) , who~~

~~established an exact relation between the Laplace transforms of i) the correlation function, ii) the chord length distribution, and iii) the surface-void correlation function (Torquato, 2002) . Despite the apparent complexity, the approach in Roberts and Torquato (1999) s involves the simplified assumption that consecutive chords on the random ray in Fig. 1a are statistically independent. Though this assumption is never strictly met, it is shown in Roberts and Torquato (1999) that this is not a practical limitation. Their relation also provides a very good approximation for correlated structures such as bicontinuous Gaussian random fields, but at the expense of the complexity from the numerical inversion of Laplace transforms.~~

To this end we ~~start from a yet simpler~~ employ a relation between the correlation function and chord length distribution that was put forward in the early stages of small angle scattering (Méring and Tchoubar, 1968) to interpret the scattering curve in terms of particle properties. In the present notation the relation can be written as

$$p(\ell) = \mu_1 \frac{d^2}{d\ell^2} A(\ell), \tag{13}$$

which was also used by Gille (2000). ~~The equation was derived for dilute assemblies of convex particles, an assumption which is not valid for snow. However,~~

Although Eq. (13) is only valid under certain assumptions which will be discussed in sec.5, it has already some non-trivial implications ~~which can be used~~ that can be exploited for the subsequent analysis.

As a first consistency check of the approximation Eq. (13), we can compute the first moment of the chord length distribution from Eq. (11) for $n = 1$, by inserting Eq. (13) and integrating by parts. This yields $\mu_1 = \mu_1 A(0)$ which is correct by virtue of Eq. (3).

As a next step, we aim at an expression for the second moment of the chord length distribution in terms of interfacial curvatures ~~according to~~ by using Eq. (11) for $n = 2$. Again, inserting Eq. (13) and integrating by parts yields

$$\mu_2 = 2\mu_1 \int_0^\infty A(r)\, dr = 2\mu_1 f(\phi, \lambda_1 \cancel{f \frac{\lambda_2}{\lambda_1}}, \lambda_2, \ldots). \tag{14}$$

~~with an unknown scaling function~~ Though f ~~. To motivate the second equality in we note that the expansion implies that $A(r)$ depends at least on two independent length scales,~~ is an unknown function here, this link shows that the chord length metric μ_2 must be somehow related to the correlation function metrics λ_1 and λ_2. ~~As a dimensionless quantity, $A(r)$ can only depend on (arbitrarily chosen) ratios of involves length scales. In the absence of other relevant scales, the correlation function must have the form $A(r) = A(r/\lambda_1, \lambda_2/\lambda_1)$. In turn, the integral over $A(r)$ in has units of length and must have the form $\int_0^\infty A(r) = \lambda_1 f(\lambda_2/\lambda_2)$ with an unknown function~~ In section 4 we will statistically investigate the dependence of f ~~. The representation is thus an implication of dimensional analysis.~~ on its arguments.

~~The validity of the main relation for the chord length distribution Eq. can be assessed by experimental data and the inferred connection Eq. between the second moment of the chord length distribution and interfacial curvatures will guide us in retrieving an empirical relation for the second moment μ_2 in terms of shape.~~

3 Methods

3.1 Data

For the following analysis we used an existing ~~dataset of microstructures reconstructed by~~ μCT ~~previously~~ dataset of 3D microstructure images described and used in Löwe et al. (2013) for a thermal conductivity analysis and Löwe and Picard (2015) for a comparison of microwave scattering coefficients. All samples were classified according to Fierz et al. (2009) as described in the supplement of Löwe et al. (2013). The data set comprises 167 different samples including two time series of isothermal experiments, four time series of temperature gradient metamorphism experiments and a set of 37 individual samples. In total, the set includes 62 samples of depth hoar (DH), 54 of rounded grains (RG), 33 of faceted crystals (FC) 10 of decomposing and fragmented precipitation particles (DF), 5 of melt forms (MF) and 3 of precipitation particles (PP).

3.2 Geometry from correlation functions

Obtaining the normalized correlation function $A(r)$ from a μCT image can be conveniently done by using the Fast Fourier Transform (FFT) as e.g. described in Newman and Barkema (1999). The FFT is typically used for performance issues to evaluate the convolution integral Eq. (2) since direct methods can be very slow. The spatial resolution of the correlation function depends on the voxel size Δ of the μCT image which ranges from ~~18~~ 10 to 50 μm. ~~The~~

Since the snow samples in the data set are anisotropic (Löwe et al., 2013) , the normalized correlation function is first obtained in the x, y and z direction and then averaged arithmetically over ~~these~~ the three directions i.e, $A(r) = (A_x(r) + A_y(r) + A_z(r))/3$~~, to average out anisotropy~~.

From the normalized correlation function two types of parameter fittings are performed. First, the exponential correlation length ξ is obtained by fitting the μCT data to the exponential form Eq. (4). Technically, we estimated the inverse parameter k by least-squares optimization of the model $A(r) = \exp(-kr)$ to the data in a fixed range of $0 < r < 50\Delta$. An illustration of this method is shown in Fig. 1b. In the following we denote by ξ the inverse of the optimal fit parameter $\xi := 1/k$. Second, we estimated the expansion parameters λ_1 and λ_2 of the correlation function by a least-squares regression to the expansion Eq. (5). Technically, we fitted $A(r) = 1 - k_1 r(1 - k_2 r^2)$ in the fixed range of $0 < r < 3\Delta$ which determines the derivatives at the origin. ~~In the following we denote~~ We denote by λ_1^{cf} and λ_2^{cf} ~~by~~ the inverse of the optimal fit parameters $\lambda_1^{\mathrm{cf}} := 1/k_1$ and $\lambda_2^{\mathrm{cf}} := 1/k_2$. The superscript is added to discern these correlation function based estimates from those presented in the next section for a validation. The influence of resolution and anisotropy to the estimates of λ_1 and λ_2 is discussed in section 5.

3.3 Geometry from triangulations

~~Essential for the present analysis in view of shape is the geometrical interpretation (Eq. and Eq.) of the parameters~~ To confirm the geometrical interpretation of λ_1^{cf} and λ_2^{cf} ~~obtained from the correlation function. To confirm this interpretation, and to make contact of the present method to previous work on curvature properties of the ice-air interface, we also compute~~ we use an alternative and independent method to estimate these parameters by ~~independent means.~~

~~To this end we provide alternative estimates λ_1^{vtk} and λ_2^{vtk} from a VTK-based image analysis (www.vtk.org) yielding estimates of~~ measuring the surface area and ~~local curvatures via triangulation~~ the local curvatures with a VTK-based image analysis as described in Krol and Löwe (2016). In short, a triangulated ice-air interface is obtained by applying ~~a~~ the VTK-Contour filter. After this step, the interface still resembles the underlying voxel structure. Therefore, in a second step the triangulated interface is smoothed by applying the VTKSmoothing filter which involves a smoothing parameter S which is the number of iterations a Laplacian smoothing on a mesh is repeated. For further details ~~see~~ we refer to Krol and Löwe (2016).

3.4 Accuracy of surface area and curvatures estimates

The measured total surface area is obtained by integrating (summing) the surface area of the triangles over the surface and the estimate λ_1^{vtk} which naturally depends on the smoothing parameter. A comparison of the triangulation and the correlation function based length scale is shown in Fig. 2 (middle row). A higher value of the smoothing parameter implies a lower surface area s (caused by shrinking of the enclosed volume upon smoothing) and in turn higher estimates for λ_1^{vtk}. Using higher smoothing also results in a higher variance in the data. This is likely due to filtering of small perturbations in the surface causing the individual samples to react differently.

It is illustrative to ~~show~~ note that even without smoothing for $S = 0$ the obtained triangulated surface is still different from the voxel surface s_{mf}, which is obtained by the union of ice-air transition faces in the voxel based image (as illustrated by the red contour in Fig. 1a). The quantity s_{mf} is one of the four Minkowski functionals and can be computed by standard counting algorithms (Michielsen and Raedt, 2001). For isotropic systems, and statistically representative samples, the relation between the surface obtained from the correlation function $s_{\mathrm{cf}} = 4\phi(1-\phi)/\lambda_1^{\mathrm{cf}}$ and the Minkowski functionals is known to be $s_{\mathrm{cf}} = 2s_{\mathrm{mf}}/3$ as discussed ~~Scatter plot of the averaged interfacial area obtained by the the correlation function method s_{cf} versus Minkowski functionals method s_{mf}.~~ in Torquato (2002, p. 290)~~and shown here in Fig. ??~~.

An estimate for the ~~curvature length~~ curvature-length λ_2^{vtk} is obtained from the VTKCurvature filter on the triangulated ice-air interface yielding local values for mean and Gaussian curvature which can be integrated to compute λ_2^{vtk} via Eq. (8). The comparison of the triangulation based ~~curvature length~~ curvature-length and the correlation function based curvature length is shown in Fig. 2 (bottom row). ~~The parameters λ_1^{vtk} and~~ Again, λ_2^{vtk} ~~depend~~ depends strongly on the smoothing parameter S. The value $S = 200$ performed best by comparing the value ~~λ_2^{vtk}~~ λ_2^{cf} to λ_2^{vtk}, see Fig. 2 (bottom row). The deviations from the 1:1 line are caused by the overestimation of the curvatures by the remaining steps in the triangulation from the underlying voxel-based data, and is thus anti-correlated with the size of the structures and the resolution. In the end, we chose a smoothing parameter $S = 200$ that is, on average, acceptable for all involved samples.

Overall, the comparison provides reasonable confidence that the geometrical interpretation of the correlation function parameters is correct, though uncertainties inherent to the smoothing operations must be acknowledged. In the following we solely use the quantities derived from the correlation function, viz. $\lambda_1 = \lambda_1^{\mathrm{cf}}$ and $\lambda_2 = \lambda_2^{\mathrm{cf}}$ where the superscripts are omitted for brevity.

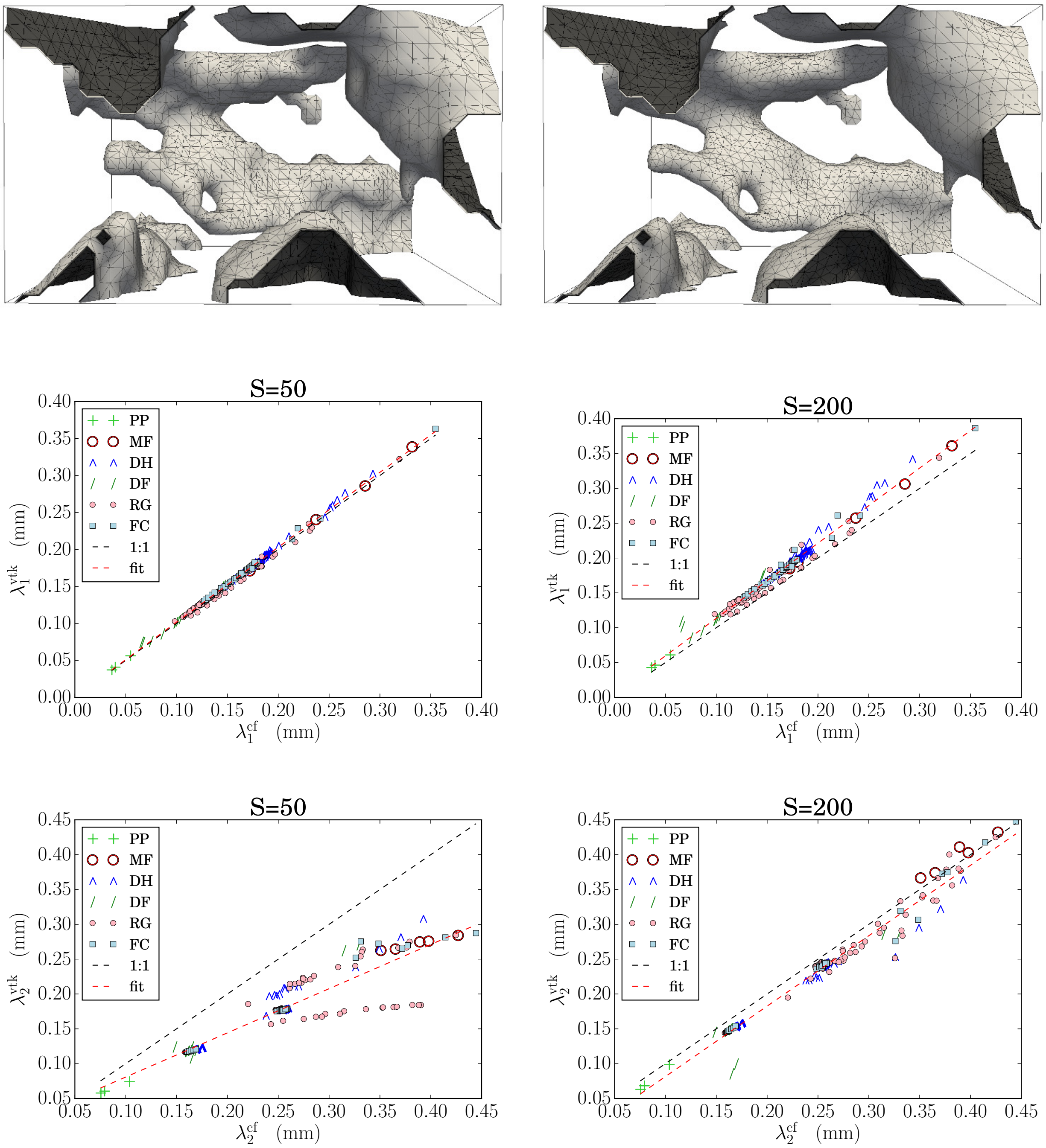


Figure 2. Comparison between smoothing paramater $S = 50$ (left) and $S = 200$ (right) for the top: Representation of the surface of a subsection of a snow sample. In the middle: Scatter plots of the ~~correlation~~ Porod length λ_1^{cf} versus λ_1^{vtk}, including a fit (red dotted line). At the bottom: Scatter plots of the ~~curvature length~~ curvature-length λ_2^{cf} versus λ_2^{vtk}, including a fit (red dotted line).

3.5 Chord length distribution

To compute the ice chord length distribution from the binary images, *all* linear lines through the sample in all three Cartesian directions $\beta = x, y, z$ are considered and *all* ice chords were measured and binned to obtain direction dependent counting densities $n^\beta(\ell)$. Here $n^x(\ell)$ denotes the total number of chords in x direction which have length ℓ. For a binary CT image, ℓ can take integer values $0 < \ell < L_x$ which are restricted by the sample size $L_x = N_x\Delta$ and the voxel size Δ of the image. The mean chord length and other moments μ_i are then computed from

$$\mu_i = \frac{1}{\sum_{\ell,\beta} n^\alpha(\ell)} \sum_{\ell,\beta} \ell^i n^\beta(\ell) \tag{15}$$

3.6 Statistical models

~~A~~ The main part of the following analysis comprises statistical relations between the length scales derived from the chord length distribution and the correlation function in section 2. In total, we will consider a few statistical models that first relate the exponential correlation length ξ and μ_2 to the geometrical length scales λ_1 and λ_2 and second, relate ξ to μ_1 and μ_2. We will start with a one-parameter statistical model and compare the results to the two parameter models. We will assess and compare the quality of the fits with the adjusted correlation coefficient R^2.

4 Results

4.1 Relating exponential correlation length to ~~optical diameter~~the Porod length and curvature-length

As a starting point for the statistical analysis we revisit the empirical relation

$$\xi = 0.75\lambda_1, \tag{16}$$

which is equivalent to Eq. (1) by virtue of Eq. (7), as suggested by Mätzler (2002). To this end we fitted ξ and λ_1 and obtained an average slope of 0.79 with a correlation coefficient of $R^2 = 0.733$, shown by the green dashed line in Fig. 3a. In the next step we fitted the same data to include an intercept parameter

$$\xi = a_0 + a_1\lambda_1. \tag{17}$$

Here the ~~correlation coefficient~~ adjusted correlation coefficient, accounting for the inclusion of extra parameters, is $R^2 = 0.731$ and ~~and~~ the parameters are given by $a_0 = 5.93 \times 10^{-2}$ mm, $a_1 = 0.794$, with very low p-values ($p < 5 \times 10^{-4}$) for the intercept and the slope ensuring the significance of the parameters of the fit. The order of magnitude of the intercept a_0 is negligible. To understand the remaining scatter we have plotted the residuals $\xi - (a_0 + a_1\lambda_1)$ versus the curvature-length λ_2 as shown in Fig. 3b. The correlation coefficient is given by $R^2 = 0.644$ and suggest that including the curvature lengths can improve Eq. (17). For an overview, this and all other statistical models will be listed in Table 1.

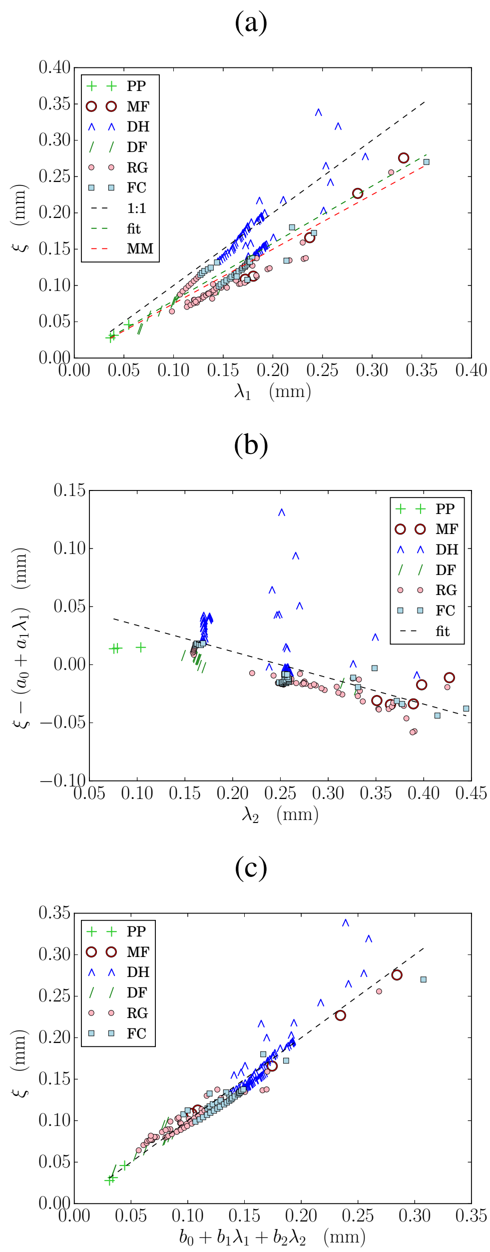


Figure 3. Scatter plots of a) the exponential correlation length ξ versus the ~~correlation~~ Porod length λ_1. A linear fit is plotted in green. Additionally the prediction of Eq. (16) (MM) is plotted in red. b) The residuals of ξ and the statistical model Eq. (17), versus the ~~curvature length~~ curvature-length λ_2. c) The statistical model Eq. (18) predicting ξ depending on the ~~optical diameter~~ Porod length λ_1 and the ~~curvature length~~ curvature-length λ_2.

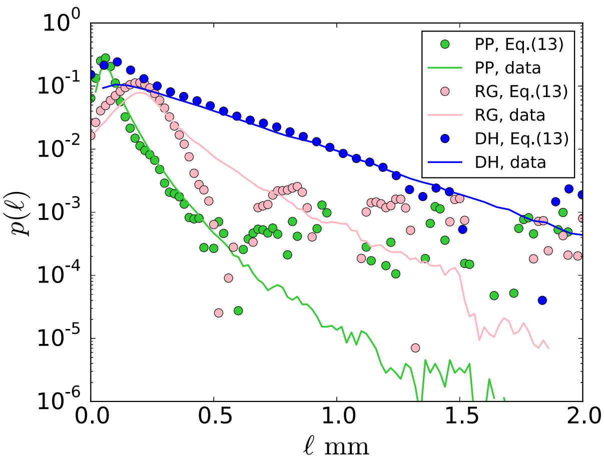


Figure 4. ~~Plot~~ Comparison of the chord length distributions computed ~~by~~ from Eq. (13) (symbols) and by direct analysis ~~, Eq.~~ of the μCT data (solid-line) for three examples of snow types (PP, RG and DH).

4.2 ~~Relating the exponential correlation length to the correlation length and curvature length~~

~~As a~~ In the next step we ~~have included the curvature length~~ include the curvature-length λ_2 ~~and~~ where we fitted the exponential correlation length ξ to the model

$$\xi = b_0 + b_1\lambda_1 + b_2\lambda_2. \tag{18}$$

The results are shown in Fig. 3c. Here we find an improvement compared to Eq. (17). The correlation coefficient is $R^2 = 0.922$ and the fit parameters are given by $b_0 = 1.23 \times 10^{-2}$ mm, $b_1 = 1.32$ and $b_2 = -3.85 \times 10^{-1}$. The p-values are very small for all coefficients b_i. The order of magnitude of the improvement can already be roughly estimated from the ratio of the prefactors b_1 and b_2. ~~To provide further evidence that the improvement of the prediction comes from the curvature length, we analyzed the residuals of the prediction Eq. and plotted~~ $\cancel{\xi - (a_0 + a_1\lambda_1)}$ ~~versus the curvature length scale~~ $\cancel{\lambda_2}$ ~~as shown in Fig. 3b.~~

~~The residuals of~~ $\cancel{\xi}$ ~~with the statistical model Eq. show a correlation with~~ $\cancel{\lambda_2}$ ~~of~~ $\cancel{R^2 = 0.644}$~~, which eventually causes the improvement for the exponential correlation length.~~

4.2 Connection between chord length distributions and correlation functions

To ~~bridge to~~ relate the chord length metrics to the Porod length and the curvature-length, we first assess the relation between the chord length distribution $p(\ell)$ and the correlation function $A(\ell)$ as suggested by Eq. (13). To this end we compared the chord length distribution obtained directly from the μCT image (cf. section 3.5) with the prediction of Eq. (13) via the correlation function for a few examples of different snow types. The results are shown in Fig. 4. The selected snow samples are the same as those used in Löwe and Picard (2015, Fig. 8 and Fig. 9). Qualitatively, the characteristic form (i.e, single maximum), the location of the maximum, and the width of the distribution are correctly predicted by Eq. (13). On the other hand, there are obvious shortcomings, such as the oscillatory tail for the RG example when the chord length distribution is derived via Eq. (15). We will revisit ~~this feature~~ these characteristics in the discussion.

4.3 ~~Second~~ Relating the second moment of the chord length distribution to the Porod length and the curvature-length

Using the previous results we can derive an approximate relation between the second moment of the chord length distribution and the interfacial curvatures. To motivate a statistical model~~we build on~~, we start from Eq. ~~, which suggests a general scaling form~~ (14),

$$\frac{\mu_2}{2\mu_1} = \lambda_1 f\left(\frac{\lambda_2}{\lambda_1} \phi, \lambda_1, \lambda_2, \ldots\right). \tag{19}$$

We investigate the ~~validity of this expression by approximating the unknown~~ dependency of the function f ~~by successively higher orders of λ_2/λ_1~~ on parameters λ_1, λ_2 and ϕ of this expression by successively including λ_1, λ_2 and ϕ in a statistical model. In a first step we approximate f by a ~~constant using the statistical model~~ statistical model including only λ_1

$$\frac{\mu_2}{2\mu_1} = l_0 + l_1\lambda_1. \tag{20}$$

~~Although not predicted by Eq. , we again allow for an interception term l_0 similar to Eq. , and Eq. .~~ The optimal parameters for ~~the~~ model Eq. (20) are $l_0 = -2.40 \times 10^{-2}$ mm and $l_1 = 1.25$, with negligible $p-$values and a correlation coefficient of $R^2 = 0.898$. The results are shown in Fig. 5a.

In view of the inclusion of the ~~curvature length~~ curvature-length λ_2, we analyzed the residuals of the previous statistical model and plotted them as a function of λ_2 (Fig. 5b). ~~We find a correlation coefficient of~~ The correlation coefficient ($R^2 = 0.295$~~, which indicates only a small benefit of~~) is small but including λ_2 in the analysis further improves the fit. The respective statistical model

$$\frac{\mu_2}{2\mu_1} = n_0 + n_1\lambda_1 + n_2\lambda_2 \tag{21}$$

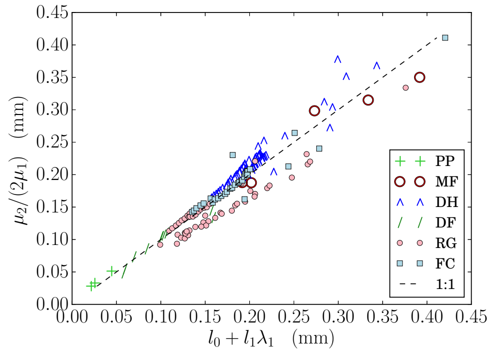
yields optimal parameters ~~$n_0 = 3.95 \times 10^{-3}$ mm~~ $n_0 = -3.95 \times 10^{-3}$ mm, $n_1 = 1.50$ and $n_2 = -2.46 \times 10^{-1}$ with a correlation coefficient $R^2 = 0.949$. The p-value for the intercept n_0 is 0.36. For n_1 and n_2 the p-values are again very low.

We have heuristically found a possibility of improving Eq. (21) even further. This was achieved by including a factor $(1-\phi)$ on the left-hand side. More precisely, we tried

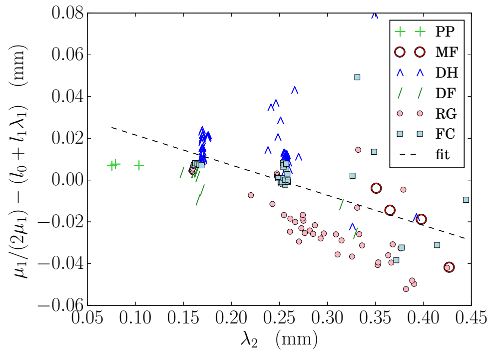
$$\frac{(1-\phi)\mu_2}{2\mu_1} = q_0 + q_1\lambda_1 + q_2\lambda_2 \tag{22}$$

as a statistical model. Here the optimal parameters are ~~$q_0 = -1.23$ mm, $q_1 = 1.03$~~ $q_0 = -1.23 \times 10^{-2}$ mm, $q_1 = 1.03$, and $q_2 = -1.98 \times 10^{-1}$. The p-values for all coefficients are negligible and the correlation coefficient is $R^2 = 0.980$. The results are shown in Fig. 5c. ~~The origin of the improvement of Eq. over Eq. is discussed in section ??.~~

(a)



(b)



(c)

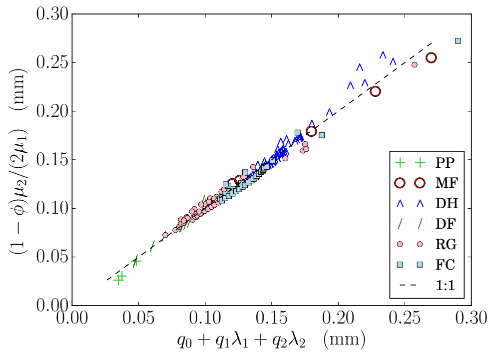


Figure 5. Scatter plots of a) the statistical model see Eq. (20) predicting $\mu_2/2\mu_1$ depending on the ~~optical diameter~~ Porod length λ_1, b) the residuals of $\mu_2/2\mu_1$ and the statistical model Eq. (20) versus the ~~curvature length~~ curvature-length scale parameter λ_2, c) the statistical model predicting $(1-\phi)\mu_2/2\mu_1$ (see Eq. (22)) depending on the ~~optical diameter~~ Porod length λ_1 and the ~~curvature length~~ curvature-length λ_2.

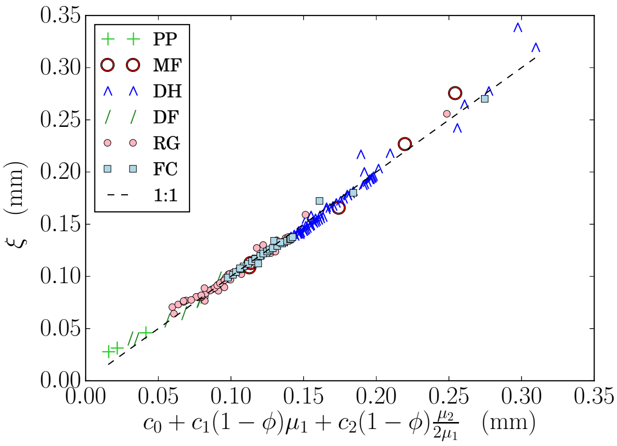


Figure 6. Scatterplot of the exponential correlation length ξ versus the statistical model Eq. (23) that depends on the first and second moment of the chord length distribution, μ_1 and μ_2.

4.4 Relating microwave metrics and optical metrics

In the previous sections we found a statistical relation between the ~~correlation length~~ exponential correlation length ξ and the geometrical ~~scales~~ lengths λ_1 and λ_2 on one hand and a relation between the ~~exponential correlation length and~~ first and second moment of the chord length ~~moments~~ distribution (μ_1 and μ_2) and λ_1 and λ_2 on the other hand. Both findings can be recast into a direct connection between the moments of the chord lengths μ_1 and μ_2 and the exponential correlation length ξ. We express this relation in the statistical model

$$\xi = c_0 + c_1(1-\phi)\mu_1 + c_2\frac{(1-\phi)\mu_2}{2\mu_1}. \tag{23}$$

Note that $(1-\phi)\mu_1 = \lambda_1$ by virtue of Eq. (12), which means that we essentially replace λ_2 by $(1-\phi)\mu_2/2\mu_1$ in the statistical model Eq. (18) that relates ξ to λ_1 and λ_2. We obtained the correlation coefficient $R^2 = 0.985$ for the optimal parameters $c_0 = 9.28 \times 10^{-3}$ mm, $c_1 = -7.53 \times 10^{-1}$, $c_2 = 2.00$. This final relation Eq. (23) significantly improves both models Eq. (17) and Eq. (18).

The summary of all models is given in Table 1. To ensure that the inclusion of an additional parameter e.g. by going from model Eq. (17) to model Eq. (18), is indeed an improvement, we have employed the Akaike information criterion (AIC) (Akaike, 1998) . The AIC measure allows to discern if the improvement of the correlation coefficient is trivially caused by an increasing number of fit parameters or an actual improvement on the likelihood of the fit due to the relevance of the added parameters. Absolute AIC-measures have no direct meaning, however a decrease of at least $2k$ between two models, where k is the number of extra parameters, implies a statistical improvement. For our case $k = 1$ the difference in the AIC-measure between Eq. (17) and Eq. (18) is 177 confirming the statistical relevance significance of λ_2.

Table 1. Summary Statistical Models

model	Eq.(#)	parameters (in order)	(adj.) R^2
$\xi = a_0 + a_1\lambda_1$	(17)	5.93×10^{-2} mm, 0.79	0.731
$\xi = b_0 + b_1\lambda_1 + b_2\lambda_2$	(18)	1.23×10^{-2} mm, 1.32, -3.85×10^{-1}	0.922
$\xi = b_0 + c_1(1-\phi)\mu_1 + c_2(1-\phi)\mu_2/2\mu_1$	(23)	9.28×10^{-3} mm, -7.53×10^{-1}, 2.00	0.985
$\mu_2/2\mu_1 = l_0 + l_1\lambda_1$	(20)	-2.40×10^{-2} mm, 1.25	0.898
$\mu_2/2\mu_1 = n_0 + n_1\lambda_1 + n_2\lambda_2$	(21)	-3.95×10^{-3} mm, 1.50, -2.46×10^{-1}	0.949
$(1-\phi)\mu_2/2\mu_1 = g_0 + g_1\lambda_1 + g_2\lambda_2$	(22)	-1.23×10^{-2} mm, 1.03, -1.98×10^{-1}	0.980

4.5 Shape factors g^G and B

As an application of the values obtained for the moments of the chord length distribution we can now compute the "shape diagram" of the optical parameters (g^G, B) suggested in Libois et al. (2013) derived from (Malinka, 2014, Eq. 60) , and Eq. (A4). The results depend on the value of the Laplace transform at the absorption coefficient α, and thus on wavelengths. For most wavelengths in the visible and near infrared regime $\alpha\mu_1 \ll 1$ is small and therefore the Laplace transform Eq. (9) can be approximated by a few terms in the expansion Eq. (10). Taking typical values for α allows us to estimate the relative importance $\alpha\mu_2/2\mu_1$ of the second-order term compared to the first-order term in the expansion Eq. (10). These values are obtained by using the values for κ provided by Warren and Brandt (2008) . The first order $\alpha\mu_1$ and ratio $\alpha\mu_2/2\mu_1$ is calculated for typical wavelengths and shown in Table 2. The values and standard deviations denote averages taken over all samples. Wavelengths are selected to match common optical methods, namely 0.9 μm (Matzl and Schneebeli, 2006) , 1.31 μm (Arnaud et al., 2011) , and the SWIR wavelengths 1.63 μm, 1.74 μm and 2.26 μm used by Domine et al. (2006) . We added the wavelength 2.00 μm, which is not used by any instrument, but has the highest value for α in this range. Note that for this wavelength $\alpha\mu_1$ is not small and the expansion of the Laplace transform, Eq. 10, likely not a good approximation. The standard deviations are high as a result of the variations due to grain type. The lowest values of $\mu_2/2\mu_1$ are found for fresh snow (PP) and highest for depth hoar (DH) and melt forms (MF).

The values in Fig. 7 for g^G and B are computed for wavelength 1.3μm and shown as a scatter plot of B versus $1-g^G$ similar to Libois et al. (2013) . The range of values for $B \in [1.54, 1.72]$ and $(1-g^G) \in [0.315, 0.335]$ is within the range $B \in [1.25, 2.09]$ and $(1-g^G) \in [0.2, 0.5]$ obtained by ray-tracing simulations for different geometrical shapes (Libois et al., 2013) . The variations of the values for different snow types is however very small. To complete the analysis we have computed g^G and B for higher absorbing wavelengths for which the shape signature might be higher, but the expansion of Eq. (10), less reliable. The results are averaged over all snow samples and included in Table 2.

Table 2. Determination of the absorption coefficient α (Warren and Brandt, 2008) , the first order, the fraction of the first and second order of Eq. (10), and the obtained estimates for B and g^{G} averaged over all snowsamples, including the standard deviation σ.

wavelength (μm)	α (m^{-1})	$\alpha\mu_1 \pm \sigma$	$\mu_2/2\mu_1\alpha \pm \sigma$ (%)	B	$1 - g^{\mathrm{G}}$
0.90	4.1	0.00094 ± 0.0003	< 0.5	1.71 ± 0.00	0.323 ± 0.000
1.31	1.2×10^2	0.026 ± 0.008	2 ± 1	1.64 ± 0.02	0.316 ± 0.000
1.63	2.0×10^3	0.45 ± 0.14	37 ± 13	0.89 ± 0.20	0.253 ± 0.011
1.74	1.1×10^3	0.24 ± 0.079	20 ± 7	1.19 ± 0.14	0.272 ± 0.010
2.00*	9.4×10^3	2.1 ± 0.68	172 ± 60	-	-
2.26	1.1×10^3	0.25 ± 0.08	20 ± 7	1.14 ± 0.13	0.240 ± 0.010

* wavelength is not used for optical measurements

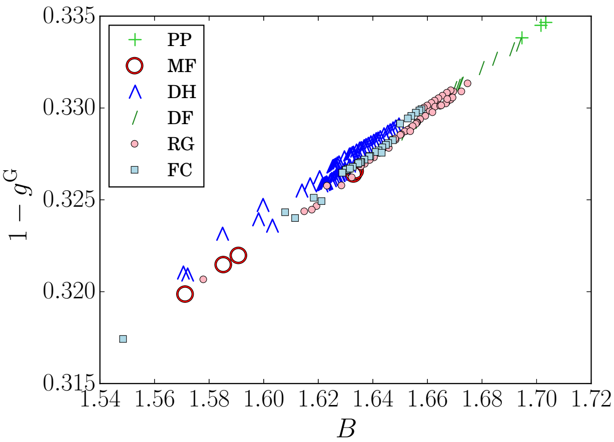


Figure 7. Scatterplot of the asymmetry factor g^{G} and the optical shape factor B evaluated for refractive index at wavelength $\lambda = 1.3\,\mu$m.

5 Discussion

5.1 ~~Retrieval of size metrics from μCT data~~Methodology

~~Retrieving geometrical properties of the ice-air interface from tomography data must be generally~~

Before turning to the discussion of physical implications of the results, we first address methodological details. Retrieving parameters from μCT images must be taken with care. In addition to the uncertainties related to filtering and segmentation pointed out by Hagenmuller et al. (2016), the present method also requires to discuss the interface-smoothing for the validation of λ_1 and λ_2, the image resolution, and the anisotropy of the samples.

5.1.1 Geometrical interpretation

The present analysis and cross-validation of ~~a~~ the curvature metric imposes ~~additional~~ requirements on the smoothness of the interface. The subtle influence of the smoothing parameter on the surface area s and averaged mean and Gaussian curvatures $\overline{H}$ and $\overline{K}$ is apparent from Fig. 2. Naturally, $\overline{H^2}$ is most sensitive to smoothing. We found a competing performance of λ_1 and λ_2 with the smoothing parameter when comparing the triangulation based estimates with the correlation function based values. The agreement for the surface area seems to be best with smoothing parameter $S = 50$. In contrast, more smoothing is ~~indeed~~ required to obtain an agreement for the ~~curvature length~~curvature-length. This higher sensitivity on the smoothing parameter is reasonable, since curvatures are defined by surface gradients which are more sensitive to a smooth mesh representation than the surface area. The competing behavior is caused by the smoothing filter, which neither preserves the volume nor the surface area of the enclosed ice upon smoothing iterations. This causes the drop in agreement for λ_1 in Fig. 2 (left, middle) with increased smoothing. As a remedy, more sophisticated smoothing filters could be used which, for example, ensure the conservation of the enclosed volume (Kuprat et al., 2001). Such problems could be partly avoided by computing normal vector fields and curvatures directly from voxel-based distance maps (Flin et al., 2005). A detailed comparison of all these different methods however, is beyond the scope of this paper. In contrast to λ_1 and λ_2, the interpretation of first and second moments of the chord length distribution, μ_1 and μ_2, is rather straightforward, where μ_1 is directly related to the optical diameter d_{opt}, and μ_2 is a measure of the variations of this size metric.

5.1.2 Resolution

Resolution plays an important role in the obtaining estimates for λ_1 and λ_2. For a μCT measurement the resolution is commonly chosen appropriately depending on snow type. While fresh Snow (PP) is typically reconstructed with $10\mu\mathrm{m}$ voxel size, melt forms (MF) and larger particles have larger voxel sizes of $35\mu\mathrm{m}$ or $54\mu\mathrm{m}$. Since we have obtained λ_1 and λ_2 with two independent methods that agree reasonably well we conclude that the resolution is generally sufficient to estimate the involved length scales. To further confirm that that there is no remaining bias with resolution we assessed the ratio $\lambda_2/\mathrm{voxelsize}$. Ideally this would be constant for all samples, implying that λ_2 is equally well resolved for all snow samples. For our data, this this ratio is 9.8 with a standard deviation of 2.6. The correlation coefficient with the voxel size is $R^2 = -.2$, which implies that there is a slight dependence on resolution. A systematic assessment is however difficult since snow types and grain sizes are not equally distributed over the resolution.

The image resolution plays another important role in the interpretation of the expansion of the correlation function. As pointed out by Torquato (2002) , a missing r^2 term is generally equivalent to a smooth interface while discontinuities, like sharp edges, would lead to a second order term. Fresh snow and depth hoar crystals are known to have these discontinuities, at least visually. But it remains questionable if these features can be detected objectively at the micrometer scale from image analysis. In an image, discontinuities are always smeared out, virtually contributing to the third order term.

5.1.3 Anisotropy

The present data set of snow samples embodies a large number of anisotropic samples, which was specifically the subject of Löwe et al. (2013) the data is based on. It is thus necessary to elaborate the impact of anisotropy on the present analysis which is exclusively involves isotropic correlation functions. It is important to note that the our analysis does not *assume* isotropy, but it rather includes the orientational averaging in the three Cartesian directions as a part of the method. Such a procedure is principally valid for arbitrary samples. Moreover, also the geometrical interpretation of the quantities remains valid. This was rigorously shown for λ_1 Berryman (1998) which relates the slope of the correlation function at the origin for arbitrary anisotropic structures after orientational averaging to the surface area per unit volume s. Though we did not find a mathematical proof for the corresponding statement for λ_2, the agreement of λ_2^{cf} (obtained from the correlation function, orientationally averaged) with λ_2^{vtk} (obtained from direct computation of the interfacial curvatures) strongly suggests its validity. In addition, we assessed that the residuals between λ_2^{vtk} (where anisotropy does not play a role) and λ_2^{cf} are not correlated with anisotropy ($R^2 = .026$).

Overall, we are confident that the method can be applied to arbitrary anisotropic samples to provide orientationally averaged length scales with the correct geometric interpretation with acceptable uncertainties due to image resolution.

5.2 Linking ~~exponential correlation lengths and curvatures~~size metrics in snow

Accepting the methodological uncertainties~~discussed in the previous section~~, we shall now discuss our findings of the statistical analysis and their relevance for the interpretation of snow microstructure.

~~As a first step we have analyzed the statistical relation between~~

5.2.1 Including size dispersity to estimate the exponential correlation length

By construction, the exponential correlation length ξ must be understood as a proxy to characterize the entire correlation function with a single length scale. This single length scale contains signatures of both, properties that dominate the behavior of the correlation function for small arguments (λ_1 and λ_2) and other properties that dominate the tail-behavior of the correlation function for large arguments.

To discuss the statistical relations we found we will start with recovering Mäzler's model (Mätzler, 2002) . This statistical model covers a relation between the exponential correlation length and ~~grain size (Mätzler, 2002) which is consistent with our data. Compared to~~ the optical grain size, or in their nomenclature: the correlation length. Mäzler's model ~~that predicts~~ predicts the slope to be $a_1 = 0.75$, ~~we find a slightly higher value of $a_1 = 0.79$. This can be explained by a large number of depth hoar samples where ξ is generally higher than~~ which is an average of $a_1 = 0.8$ for depth hoar and $a_1 = 0.6$ for other snow types. This is ~~also suggested by the data from Mätzler (2002, Tab. 1) , which indicates an influence of snow type or grain shape~~ consistent with our finding $a_1 = 0.79$ since we have many depth hoar samples in the data set, suggesting that grain shape has a direct influence on the statistical relation. This influence was made quantitative by ~~the subsequent analysiswhere we found a clear improvement of the prediction of the exponential correlation length when incorporating the curvatures length as an additional size metric~~ including the curvature-length to the statistical analysis, resulting in the statistical model Eq. (18) (Fig. 3c). The quantitative improvement on the statistical model Eq. (16) by using Eq. (18) ~~or Eq.~~ is given by the increase in the correlation coefficient from $R^2 = 0.733$ to $R^2 = 0.922$.

In addition we established a new statistical relation Eq. (23) between ξ and the moments of the chord length distribution, μ_1 and ~~$R^2 = 0.985$, respectively. To ensure~~ μ_2. This model performs even better when the correlation coefficient $R^2 = 0.985$ is taken as a quality measure. We confirmed that the inclusion of an additional parameter in Eq. (18) and Eq. (23) indeed improves on eq. (16), ~~we have employed~~ by employing the Akaike information criterion (AIC) measure (Akaike, 1998). ~~This allows us to discern if the improvement~~

All statistical models showing improvements of (1) indicate that at least two different length scales λ_1 and λ_2 or μ_1 and μ_2 are required to obtain a reasonable prediction of the exponential correlation length. While λ_1 and μ_1 are both trivially related to the optical radius via Eq. (7) and Eq. (12), the two other size metrics μ_2 or λ_2 are the origin of performance increase.

This seems surprising at first sight. Why should local aspects of the interface (λ_1 and λ_2) determine the non-local decay of structural correlations (ξ)? To illustrate our explanation for this finding, we resort to a particle picture and consider a dense, random packing of monodisperse hard spheres. For such a packing, the particle "shape" is trivial and fully determined by the sphere diameter d, which determines the slope of the correlation ~~coefficient is trivially caused by an increasing number of fit parameters or an actual improvement on the likelihood of the fit due to the relevance of the added parameters. Absolute AIC-measures have no direct meaning, however a decrease of at least $2k$ between two models, where k is the number of extra parameters, implies a statistical improvement. For our case $k = 1$ the difference in the AIC-measure between Eq. and~~ function at the origin. However, also particle positions and thus the decay of correlations is fixed by d. This becomes obvious from the representation $C(r) = n v_{\mathrm{int}}(r) + n^2 v_{\mathrm{int}}(r) * h(r)$ for the correlation function for such a system at number density n (Löwe and Picard, 2015) . In this representation, the spherical intersection volume v_{int} and the statistics of particle positions $h(r)$ both depend on d. Now imagine that each sphere is deformed by a hypothetical, volume-conserving re-shape operation to an irregular, non-convex particle, which is still located at the center of the original sphere. Due to re-shaping, the parameter $\overline{H^2}$ would increase. After the re-shape, neighboring particles would overlap (on average), since their maximum extension must have been increased compared to the sphere diameter. To recover a non-overlapping configuration, all particle positions must be dilated. The latter, however, also affects the tail of the correlation function. This is exactly what we observe: the "shape of structural units" in snow, as exemplified by $\overline{H^2}$ is always correlated with the "position of the structural units" in space. We note that this particle analogy has clear limitations and only serves here to illustrate the rather abstract statistical relations between different length scales. Snow remains a bi-continuous material where individual particles cannot be distinguished.

Overall, we conclude that both, λ_2 or μ_2 can be used to significantly improve estimates of ξ when compared to optical diameter based estimates.

5.2.2 Linking moments of the chord length distributions to Porod and curvature-length

Hitherto no geometrical interpretation for the second moment μ_2 of the chord length distribution was known. Our results suggest an empirical relation, Eq. ~~is 177 and the AIC difference between models~~ (22), that involves the two geometrical length scales λ_1 and λ_2. In the following we provide supporting arguments for the link between μ_2 and λ_1 and λ_2 by discussing the relation Eq. ~~and~~ (13) between the chord length distribution and the correlation function.

The relation Eq. ~~was 275, which confirms the statistical significance of the model Eq. .~~

~~All statistical models indicate that at least two different length scales λ_1 and λ_2 or μ_1 and μ_2 are required to obtain a reasonable~~ (13) was originally raised in the context of small angle scattering long time ago (Méring and Tchoubar, 1968) and later revisited e.g. by Levitz and Tchoubar (1992) , revealing two different approximation steps. A first simplification comes from the assumption that consecutive chords on the random ray in Fig. 1 are statistically independent. This issue has been discussed in detail also by Roberts and Torquato (1999) , who established an exact relation between the Laplace transforms of the correlation function, the chord length distribution, and a surface-void correlation function based on this assumption. Their results however show that for level-cut Gaussian random fields, where this assumption is violated, the prediction of the ~~exponential correlation length . While λ_1 and μ_1 are both trivially related to the optical radius~~ chord length distribution can be still very accurate. This indicates that assuming independent chords is per se not a serious limitation. Secondly, Eq. (13) is actually an approximation for dilute systems which is generally not valid for snow.

To test the range of validity of the relation (13) for snow, we have taken three samples and computed the chord length distribution directly to compare them to the prediction of Eq. (13) as shown in Fig. 4. An obvious drawback of Eq. (13) can be seen for the rounded grains (RG) sample. Due to the quasi-oscillations in the correlation function (cf. Löwe et al. (2011)), $A(\ell)$ and its second derivative assume negative values, which would imply negative values for $p(r)$ via Eq. ~~and~~ (13). This is in contradiction to the meaning of $p(r)$ as a probability density and likely a consequence of the assumptions which are not valid for snow. Despite this obvious drawback, Fig. 4 shows that Eq. ~~, the two other size metrics~~ (13) yields three, qualitatively consistent results for different snow types where the basic features of the chord length distrbution are well predicted: First, it captures the considerable variations of the position of the maximum, the width, and decay of the chord length distribution. Second, the relation Eq. (13) predicts that the chord length distribution tends to zero for small values i.e. $p(0) = 0$ (as confirmed in Fig. 4). This is a direct consequence of a smooth interface as shown in Wu and Schmidt (1971) . Third, it leads to Eq. (14), that involves the integral over the correlation function. The latter indicated a connection between μ_2 ~~or~~ and λ_1 and λ_2~~significantly increase the performance of the statistical model. As further detailed below, both parameters can be regarded as a two possibilities of defining~~ , which was confirmed quantitatively via Eq. (21). Given the assumptions discussed above, it is not surprising that a heuristic improvement could be achieved by including a term $(1-\phi)$ in Eq. (22), since snow is not a dilute particle system and corrections containing ϕ-terms are to be expected.

Overall, our analysis confirms that both approaches to microstructure characterization, via correlation functions (with metrics λ_1, λ_2) or via chord length distribution (with metrics μ_1, μ_2) are not independent. They rather describe, slightly different but interrelated, structural properties which are now discussed in view of grain shape.

5.3 ~~The notion of grain~~ Grain shape

5.3.1 Grain shape, a geometrical interpretation

The international classification for seasonal snow on the ground (Fierz et al., 2009) considers grain shape as the morphological classification into snow types. This is motivated by the common but loose perception of shape as the basic geometrical form of constituent particles. It is clear that grain shape remains a vague concept unless it is formulated in terms of quantities which are unambiguously defined on the 3D microstructure.

Local curvatures are often regarded as shape parameters and used to characterize snow on a more fundamental level. The relevance of the mean curvature is described and analyzed in detail in Calonne et al. (2015), where morphological transitions (e.g, faceting) of snow during temperature gradient metamorphism are visible in the distribution of mean curvatures. The present description of grain shape in snowpack models (Lehning et al., 2002; Vionnet et al., 2012) is in fact based on the variance of the mean curvature, by the ~~"sphericity " parameter as introduced by Brun et al. (1992) . There are~~ sphericity parameter as defined by Lesaffre et al. (1998) . There were attempts to measure the sphericity from digital photographs as described by Lesaffre et al. (1998) and Bartlett et al. (2008). This definition is valid only in two dimensions and therefore difficult to compare directly to their 3D counterparts in Calonne et al. (2015). ~~Another aspect of shape is captured by the averaged Gaussian curvature~~

It is therefore natural to use objective measures as the mean and Gaussian curvature $\overline{H}$ and $\overline{K}$ to quantify shape. Though $\overline{K}$ is computed from local properties of the interface, it has a strict topological meaning due to its relation to the Euler characteristic ~~χ via Eq. .~~ which is by definition strictly independent of local shape variations of the ice-air interface. The Euler characteristic was e.g. used by Schleef et al. (2014) to characterize microstructural changes during densification. ~~As a topological quantity, χ is by definition strictly *independent* of local (shape) variations of the ice-air interface.~~ We found however, that the contribution $\overline{K}/3$ in λ_2 from Eq. (8) ranges from 1-13% and is on average 3.7 % of $\overline{H^2}$. Hence the ~~curvature length~~ curvature-length λ_2 is dominated by the second moment $\overline{H^2}$, and thus closely related to the variance of an (inverse) size distribution, the distribution of mean curvatures~~, which is a well-defined shape concept for the 3D microstructure.~~ . This indicates the formal similarity to μ_2 which is also a second moment of a size distribution, the chord length distribution. Hence, both metrics can be regarded as accounting for size dispersity in snow.

~~There is a conceptual pitfall associated with shape metrics of~~ Overall, we suggest that both parameters, μ_2 and λ_2 can be used to objectively define a grain shape for 3D microstructures ~~. To illustrate this , we consider a~~ which is closely connected to size dispersity and which naturally extends grain size (optical diameter) determining μ_1 or λ_1. With this perception, we now connect back to the original applications of microwave and optical modeling.

5.3.2 Grain shape for microwave modeling

Thus far, the exponential correlation length ξ as a key parameter for MEMLS based microwave modeling (MEMLS) was mainly predicted from the optical diameter. Our conclusions from section 5.2.1 could now be restated: The inclusion of a grain shape parameter, λ_2 or μ_2 improves the prediction of the exponential correlation length significantly. Or, according to the conclusion from the previous section, one may alternatively restate that size dispersity has an influence on microwave properties. This is known from other models than MEMLS, where an influence of polydispersity on the effective grain scaling parameter within DMRT-ML microwave modeling was found Roy et al. (2013) .

This equivalence of shape and size dispersity at the level of correlation functions can be further illustrated by an interesting example. Consider a microstructure of polydisperse spherical particles. The definition of grain shape from the classification (Fierz et al., 2009) would assign a spherical shape to this microstructure, while the averaged squared mean curvature $\overline{H^2}$ would ~~be rather governed by~~ instead vary depending on the variance of particle radii. ~~This indicates that polydispersity must also be considered as a particular aspect of shape. The equivalence between polydispersity and shape can be made more rigorous as~~ As pointed out by Tomita (1986)~~: a low-density assembly of irregularly shaped but identical~~ , for low density, such a system of polydisperse spherical particles can always be mapped uniquely ~~,~~ onto an assembly of monodisperse but irregularly shaped particles by solving an integral equation, ~~onto a system of polydisperse spherical particles *if*~~ if only the correlation function is considered. ~~Irregularity~~ Shape can be equivalent to polydispersity~~. Hence,~~ , and snow types which ~~can be clearly discerned visually~~ are visually very different might still have very similar physical properties. ~~Shape must be generally understood as a distribution of size metrics. This~~ This example also explains why the ~~objectively defined shape parameter~~ objective size dispersity parameters λ_2 or μ_2 cannot be mapped ~~directly~~ onto the classical definition of grain type from Fierz et al. (2009).

5.4 ~~Linking optical and microwave metrics~~

5.3.1 Grain shape in geometrical optics

Finally, we turn to the implications of ~~different descriptions of grain shape for modeling microwave scattering or geometrical optics in snow~~size dispersity or grain shape on geometrical optics within the scope of (Malinka, 2014) based on chord length distributions.

~~The exponential correlation length must be understood as a proxy to characterize the entire correlation function by a single length scale.By construction, this single length scale contains signatures of both,~~ As pointed out by (Malinka, 2014) , if consecutive chords were statistical independent i.e. a Markovian process, then the obtained distribution would be exponential, and all optical properties solely determined by the optical diameter (or μ_1). To quantify the deviation from an exponential chord length distributions we calculated the fraction $\mu_2/2\mu_1^2$ which is unity for a exponential chord length distribution. This fraction is on average 0.75 for rounded grains (RG), 0.76 for melt forms (MF), 0.77 for precipitation particles (PP) and defragmented particles (DF), 0.79 for faceted crystals (FC) and the closest value to unity is 0.876 for depth hoar (DH). This implies that the chord length distribution for depth hoar is closest to an exponential, which can be visually confirmed by Fig. 4. We reach a similar conclusion for the correlation function where λ_1 is already a fairly good predictor for the exponential corrrelation length when depth hoar is considered (see Fig. 3)a). But due to the deviations from an exponential, an influence of shape via μ_2 on the optical properties ~~that dominate the behavior of the correlation function for small arguments (λ_1 and λ_2)and other properties that dominate the tail-behavior of the correlation function for large arguments. Within the scope of such a single length scale metric, we found clear evidence from the statistical relation Eq. that the tail is already largely determined by properties of the correlation function at the origin (λ_1 and λ_2). This seems surprising at first sight. Why should~~

~~local aspects of the interface (λ_1 and λ_2)determine the (non-local) decay of structural correlations (ξ)relevant for microwave scattering? To illustrate our explanation for this finding, we resort to a particle picture and consider a dense, random packing of monodisperse hard spheres. For such a packing, the particle "shape" is trivial and fully determined by the sphere diameter d, which determines the slope of the correlation function at the origin. However, also particle positions and thus the decay of correlations is fixed by d. This becomes obvious from the representation $C(r) = nv_{\mathrm{int}}(r) + n^2 v_{\mathrm{int}}(r) * h(r)$ for the correlation function for such as system at number density n (Löwe and Picard, 2015) . In this representation, the spherical intersection volume v_{int} and the statistics of particle positions $h(r)$ both depend on d. Now imagine that each sphere is deformed by a hypothetical, volume-conserving re-shape operation to an irregular, non-convex particle, which is still located at the center of the original sphere.Due to re-shaping, the parameter $\overline{H^2}$ would increase. After the re-shape, neighboring particles would overlap (on average), since their maximum extension must have been increased compared to the sphere diameter. To recover a non-overlapping configuration, all particle positions must be dilated. The latter, however, also affects the tail of the correlation function . This is exactly what we observe: the "shape of structural units" in snow, as exemplified by $\overline{H^2}$ is always correlated with the "position of the structural units" in space. We note that such a particle analogy has clear limitations and only serves here as an attempt to illustrate the rather abstract statistical relations between different length scales. They must be taken with caution, since snow is a bicontinuous material if probed by μCT, and individual particles cannot be distinguished.~~would be expected from Malinka (2014) .

~~The previous analogy also helps to understand why geometrical optics of snow should be related to microwave scattering, despite the difference in wave lengths by orders of magnitude. For snow optics, it has been shown that shape influences the penetration of light (Libois et al., 2013) . The authors conclude that acollection of spheres cannot sufficiently predict irradiance profiles in snow due the underestimation of the asymmetry factor g^G. This factor is known to include shape of different grain types as predicted by the theory from Kokhanovsky and Zege (2004) . However an expression of the shape parameter B in terms of the microstructure is not provided by the theory. The analysis of Malinka (2014) shows that the optical properties can be expressed in terms of the Laplace transform $\widehat{p}(\alpha)$ of the chord length distribution, which has to be evaluated at the absorption coefficient of ice, $\alpha = 2\pi\kappa/\lambda$, where λ is the wavelength and κ the imaginary part of the refractive index. Determination of the absorption coefficient α (Warren and Brandt, 2008) and the fraction of the first and second order of Eq. including the standard deviation σ.~~ Using the chord length distributions we were able to calculate the shape factors B and g^{G} from Malinka (2014) and Libois et al. (2013) in the limit of low absorption where both approaches can be compared. The (B, g^{G}) shape diagram (cf. Fig 1.(a) in Libois et al. (2013)) in Fig. 7 was obtained for wavelength ~~(μm) α (m^{-1}) $\overline{\mu_2/2\mu_1}\alpha$ (%) σ (%)~~
~~0.90 4.1 7.6×10^{-2} 2.6×10^{-2}~~

~~1.31 1.2×10^{2} 2.1 7.2×10^{-1}~~

~~1.63 2.0×10^{3} 37 13~~

~~1.74 1.1×10^{3} 20 6.8~~

~~2.00* 9.4×10^{3} 1.7×10^{2} 60~~

~~2.26 1.1×10^{3} 20 7~~

~~Since for most wavelengths in the visible and infrared regime $\alpha\mu_1 \ll 1$ is small, the Laplace transform Eq. can be approximated by a few terms in the expansion Eq. . The results in Malinka (2014) are mainly based on the Laplace transform of an exponential, $\widehat{p}(\alpha) = 1/(1+\mu_1\alpha)$, which only involves μ_1 (or the optical radius via Eq. 1) . Assessing typical values for α allows us to estimate the relative importance $\alpha\mu_2/2\mu_1$ of the second-order term compared to the first-order term in the expansion~~ 1.3 μm where the Laplace transform Eq. (10) ~~. Typical values for α are obtained by using the values for κ provided by Warren and Brandt (2008) . The ratio $\alpha\mu_2/2\mu_1$ is calculated for typical wavelengths and shown in Table 2.Wavelengths are selected to match common optical methods, namely 0.9 μm (Matzl and Schneebeli, 2006) , 1.31 μm (Arnaud et al., 2011) , and the SWIR wavelengths 1.63 μm, 1.74 μm and 2.26 μm used by Domine et al. (2006) . We added the wavelength 2.00 μm, which is not used by any instrument, but has the highest value for α in this range. Note that the standard deviation σ is high as a result of the variations due to grain shape. The lowest values of $\mu_2/2\mu_1$ are found for fresh snow (PP) and highest for depth hoar (DH) and melt forms (MF). Given the order of magnitude, it seems likely that shape corrections could be measured by some SWIR based optical techniques. To confirm the relevance of the shape correction from a different perspective, we can directly compute the optical shape parameter~~ can be approximated by the first and second order. The variations of the absolute values for B, g^{G} shown in Fig. 7 predominantly stem from corrections which are linear in μ_1 (by virtue of (A5)), while the small, scattered deviations from a perfect straight line are caused by μ_2. If B ~~in terms of μ_1, μ_2. It is straightforward to derive an expression~~ and g^{G} were evaluated for wavelength 0.9 μm, the influence of μ_2 would be even smaller. Our results show that the values for ~~B using (Libois et al., 2013; Malinka, 2014) as shown in the Appendix A. The results Scatterplot of the dimensionless quantity $\mu_2/2\mu_1^2$ and the optical shape factor B evaluated for refractive index at wavelength $\lambda = 1.3\,\mu$m. are shown in Fig. 7 where B is shown as a function of the dimensionless quantity $\mu_2/2\mu_1^2$ which can be constructed from the two relevant parameters. The range of values $B \in [1.54, 1.72]$ is well within the range $B \in [1.25, 2.09]$ obtained by~~ B and g^{G} are exactly within the range that is suggested by ray-tracing ~~calculations for different geometrical shapes (Libois et al., 2013) . Further details remain to be elucidated by combining tomography imaging together with optical measurements or pore scale simulations. Along these lines our results suggest a new route of assessing the remaining discrepancies in ? using the moments of the chord length distribution.~~ simulations for various geometrical shapes for a wavelength of 0.9 μm Libois et al. (2013) , but show a much smaller variation over the entire set of snow samples. Comparing our results to ray-tracing of geometrical shapes is however not straightforward, since the 3D microstructures cannot be mapped on an ensemble of regular geometrical objects.

~~The established connection between μ_2 and shape(via λ_2) is demonstrated by the statistical model Eq. and the residual analysis (Fig. 5). Together with the relation between ξ and λ_2 discussed in 5.2.1, we have finally established a connection between all involves size metrics. This leads to the statistical relation Eq. , which involves density, the microwave metric ξ and the optical metrics~~ If the obtained values for B are compared to actual measurements (Libois et al., 2014) also a larger variation is observed than predicted from the geometrical optics framework Malinka (2014) . It should be noted however that, as the authors discuss, the correlation between the experimentally obtained B and shape, as defined by Fierz et al. (2009) , is statistically not significant and variations might be attributed to shadowing effects relevant at higher densities.

Overall, our analysis indicates a smaller variation of optical properties with shape via μ_2 according to Malinka (2014) when compared other methods. We can only hypothesize potential origins which are connected to the present analysis. A crucial assumption made in the geometrical optics framework (Malinka, 2014) is the statistical independence of the chord length and ~~μ_1.~~

~~The statistical relations between all the size metrics was motivated by the connection between chord length distributions and correlation functions. This connection is an old topic which was raised in the context of small angle scattering half a century ago (Méring and Tchoubar, 1968) . The approximation Eq. used here actually contains two different approximation steps. A first simplification comes from the assumption that consecutive ice chords are statistically independent. Such an approximation was used by Roberts and Torquato (1999) to derive an exact, but more complicated, relation between the Laplace transforms of the ice chord length distribution and the correlation function. A similar result was obtained by Levitz and Tchoubar (1992) . The used relation Eq. underlies even an additional approximation of strong dilution of the inclusion particles (Méring and Tchoubar, 1968) . Despite the two-step approximation outlined above, we however confirmed that Eq. has a practical value and yields three, qualitatively consistent results for different snow types (Fig. 4). First, it captures the considerable variations of the position of the maximum, the width, and decay of the chord length density function. Second, it leads to the suggested Eq. which indicates that moments of the chord length distribution and the second derivative of the correlation function must be related. An heuristically found improvement on Eq. by including the term $(1-\phi)$ in Eq. is not surprising since snow is not a dilute particle system and corrections containing ϕ-terms must be expected. Third, the relation Eq. predicts that the chord length distribution tends to zero for small values i.e. $p(\ell = 0) = 0$ (as confirmed in Fig. 4) . This is a direct consequence of a smooth interface as shown in Wu and Schmidt (1971) . The latter work also derived~~ the ~~real space expansion of the~~ consecutive ice-air incidence angle for a ray which passes through a grain. Such an assumption might be progressively violated for lower absorption where a higher number of internal reflections in fact probes this assumption more often. Hence the true effect of shape on B and g^{G} might be still more pronounced as captured by size dispersity via μ_2 within (Malinka, 2014) . Further details on the discrepancies between measurements, simulations and theory remain to be elucidated by combining tomography imaging and shape analysis together with optical measurements and ray-tracing simulations in the future.

6 Conclusions

We have analyzed different microstructural length scales (λ_1, λ_2 and μ_1, μ_2) which were derived from the correlation function and chord length distribution~~which can be written as $p(\ell) = 6\ell/\lambda_2^2 + \mathcal{O}(\ell^3)$. This result based on the assumption of a dilute suspension of identical, randomly oriented particles, can be taken as an independent confirmation that the variance of the chord length distribution $\mu_2 - \mu_1^2$ must be related to the interfacial curvatures via λ_2. Under the minimal assumption that the chord length distribution is governed by at least two independent length scales , the width of the distribution must result from a competition of the rate at which the probability increases for small arguments ℓ (equal to $6/\lambda_2^2$) and the rate at which probability density decays to zero for large arguments ℓ (which must contain the optical radius~~, respectively. All length scales have a well-defined geometrical meaning. While the first order quantities (μ_1, λ_1) ~~.~~ are both related to the mean size (optical equivalent diameter), their higher order counterparts (λ_2, μ_2) are objective measures of size dispersity present in the snow microstructure. ~~.~~

~~An obvious drawback of Eq. is, however, also revealed by Fig. 4 for the RG snow . Due to the quasi-oscillations in the correlation function(cf. (Löwe et al., 2011)), $A(\ell)$ and its second derivative assume negative values, which would imply negative values for $p(r)$ via Eq. . This is in contradiction to the meaning of $p(r)$ as a probability density. The results from Roberts and Torquato (1999) for similar systems of oscillatory correlation functions indicate that the more sophisticated approach using numerical Laplace inversion seems to be a remedy, however this is beyond the scope of the present work.~~

~~As a convenient side product of our analysis, we obtained an approximate relation for the~~ For the correlation function, the length scale λ_2 is essentially determined by the second moment of the mean curvature distribution. For the chord lengths, μ_2 is the second moment of ~~μ_2 of~~ the chord length distribution~~in terms of the curvature length λ_2 (predominately via $\overline{H^2}$). The parameter $\overline{H^2}$ has also been used for shape recognition in stereology for a long time and can be obtained from particular vertex and edges counting algorithms, as shown by **?** and **?** . An analytical relation between the chord length distributions and curvatures was, however, never derived. Due to the lack of closed form expression for~~ . Both quantities naturally extend the concept of mean grain size as covered by the optical equivalent diameter. The statistical relation established between (λ_1, λ_2, μ_1, μ_2~~, our results may be relevant also for other applications~~) indicates that practically the two measures of size dispersity can be used interchangeably.

7 ~~Conclusions~~

~~In this work we have we analyzed snow microstructure and suggested a size metric which objectively, but not uniquely, characterizes shape from the expansion of the correlation function in terms of interfacial curvatures. We have shown that the geometrical interpretation of the shapeparameter is indeed correct by a comparison to VTK-based triangulation methods. This also highlighted the remaining difficulties when processing the ice-air interface, such as smoothing. Independent of these difficulties, the shape analysis allowed us to improve~~ We have argued that size dispersity is one possible route towards an objective definition of grain shape, and thus both quantities (λ_2, μ_2) can be regarded as measures of shape. Within this interpretation, we found that grain shape or size dispersity significantly improves a widely used statistical model for the exponential correlation length (as a key size metric for MEMLS based microwave modeling)~~from the optical radius by including shape via curvatures. Alternatively, the exponential correlation length can also be expressed in terms of moments of the chord length distribution (as the key metric for geometrical optics modeling). We analyzed the connection between chord length distributions and correlation functions which was suggested by old arguments from small angle scattering. Loosely speaking, the established connection states that local shape of irregular snow grains (determining optical response via the chord lengths or curvatures) and the packing of these irregular grains (determining microwave response via the correlation length)is intimately correlated. Our results suggest a new experimental route to connect optical in-situ field measurements with microwave measurements. This requires to design an experimental method which is able to retrieve the μ_2 corrections (shape)~~

~~in the optical properties when compared to the μ_1 term (optical radius). This seems possible given the predicted values for the optical shape factor~~ .

We have also used this interpretation of shape to assess the so called optical shape factor B ~~. In a second step, using the statistical relation Eq. , a direct connection to the correlation length can be made. Even by treating snow here as an isotropic medium (by averaging all quantities over directions) we have found statistically robust relations between all size metrics. With ongoing progress in models for the correlation function that include anisotropy and more general forms other than exponential ones, we can expect further refinement in the relation between optical and microwave metrics in the future~~which can be related to μ_1 and μ_2 in the framework of Malinka (2014) . The results suggest that size dispersity is only a first, but likely not a complete step to characterize shape for optical modeling.

Overall, defining grain shape via dispersity measures μ_2 or λ_2 provides a clear intersection between microwave modeling of snow (if based on the exponential correlation length) and optical modeling of snow (if based on Malinka (2014)). We do not believe this intersection to be exhaustive: The influence of shape in snow optics likely involve more than size dispersity. And size dispersity is likely not sufficient to explain the full diversity of microwave properties of snow. But the established overlap of relevant microstructure parameters provides a clear quantitative starting point for further improvements.

Appendix A: Optical shape factor B from moments of the chord length distribution

To derive an expression of the optical shape factor B in terms of the moments of the chord length distribution, we start from expression (Libois et al., 2013, Eq. 6) for the single scattering co-albedo ~~$(1-\omega)$ as defining equation~~

$$(1-\omega) = B\,\frac{\gamma V}{2\Sigma}\,, \tag{A1}$$

which ~~relates B to~~ is related to B, the average volume of a particle V, the average projected area of a particle Σ, and the absorption coefficient γ. This can be ~~reformulated in the~~ recast in terms of the mean chord-length ~~picture by using (Malinka, 2014, Eq. 6) . Then,~~ using (Malinka, 2014, Eq. 6) , which yields, adopting the notation of the present paper, the relation ~~can be written as~~

$$(1-\omega) = B\,\frac{\alpha\mu_1}{2} \tag{A2}$$

~~Using the expression of~~ On the other hand, an expression for the single scattering ~~albedo from Malinka (2014, Eq. 56) , inserting~~ co-albedo is directly provided by Malinka (2014, Eq. 56) . Inserting (Malinka, 2014, Eq. 29,42,49,18) and re-arranging terms we obtain

$$(1-\omega) = \frac{T_{\mathrm{out}}(n)}{1+\dfrac{T_{\mathrm{out}}(n)}{n^2}\,\dfrac{\widehat{p}(\alpha)}{1-\widehat{p}(\alpha)}} \tag{A3}$$

in terms of the real part of the refractive index n, the averaged Fresnel transmittance coefficient $T_{\mathrm{out}}(n)$ (given by Malinka (2014, Eq. 19) in closed form) and the Laplace transform of the chord length distribution $\widehat{p}(\alpha)$. ~~By comparing~~

To obtain an expression for B by comparing Eq. (A2) and Eq. (A3) ~~, and taking~~ it must be noted that both expression are based on slightly different assumptions. While Eq. (A1) is meant to be valid only in the limit of low absorption (Libois et al., 2013) , Eq. (A3) is valid for arbitrary values of α. This is reflected by the existence of the limit $\alpha \to \infty$ in Eq. (A3), while Eq. (A2) diverges if B is regarded as a constant which is strictly independent of α. Hence the comparison of Eq. (A2) and Eq. (A3) must be limited to small values of $\alpha\mu_1$ in order to obtain an expression for B which can be compared to the results from (Libois et al., 2013) . That said, we equate Eq. (A2) and Eq. (A3), take into account an additional factor of 2 between ~~(Malinka, 2014) and (Libois et al., 2013)~~ Malinka (2014) and Libois et al. (2013) due to a different treatment of the extinction efficiency, we end up with

$$B = \frac{1}{\alpha\mu_1} \frac{T_{\mathrm{out}}(n)}{1 + \dfrac{T_{\mathrm{out}}(n)}{n^2} \dfrac{\widehat{p}(\alpha)}{1-\widehat{p}(\alpha)}} \tag{A4}$$

Complemented by the approximation Eq. (10) for the Laplace transform $\widehat{p}$, the expression (Malinka, 2014, Eq. 19) for $T_{\mathrm{out}}(n)$, this yields an expression of the shape factor B in terms of the first and second moment, $\cancel{\mu_1, \mu_2}$ μ_1 and μ_2, of the chord length distribution, the real part of the refractive index n and the absorption coefficient α.

To explicitly reveal the correction of B for small α which involves the second moment of the chord-length distribution, we expand Eq. (A4) around $\alpha = 0$ to obtain

$$B = n^2 \left[1 - (\alpha\mu_1) \left(\frac{n^2}{T_{\mathrm{out}}(n)} - 1 + \frac{\mu_2}{2\mu_1^2} \right) \right] \tag{A5}$$

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